THE DYNAMIC EFFECT IN THE HYDROBORATION OF ALKENES

A Dissertation

by

YATSANDRA OYOLA

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

December 2010

Major Subject: Chemistry

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Approved by:

Chair of Committee,	Daniel A. Singleton
Committee Members,	Frank M. Raushel
	David E. Bergbreiter
	Cesar Malave
Head of Department,	Simon W. North

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ABSTRACT

The Dynamic Effect in the Hydroboration of Alkenes. (December 2010)

Yatsandra Oyola, B. S., University of Puerto Rico

Chair of Advisory Committee: Dr. Daniel A. Singleton

The hydroboration of simple alkenes with BH_3 preferentially occurs in an anti-Markovnikov fashion. The standard explanation for this preference, reproduced in all general organic chemistry textbooks, is that the selectivity arises from a greater stability for the anti-Markovnikov transition state. This explanation presupposes the applicability of the transition-state *theory model* for reactivity and selectivity. This dissertation explores the applicability of transition state theory to selectivity in hydroborations and finds that in some cases transition state theory fails to accurately account for observations.

Experimental results for the hydroboration of propene-d_6 and styrene-d_8 with excess BH_3 was analyzed by ^{2}H-NMR to determine the percentage of the Markovnikov product for the BH_3-mediated reaction. The experimental selectivities were then compared with predictions based on very high-level calculations using transition state theory. It was observed that the regioselectivity of the hydroboration of these alkenes is lower than can be accounted for by transition state theory. The regioselectivity discrepancy was explored through dynamic trajectory analysis.

It is proposed here that the observed regioselectivity is that of a "hot" reaction, resulting from an exothermic association of alkene with borane to form an intermediate complex. This complex then overcomes low-energy barriers to form anti-Markovnikov and Markovnikov products faster than excess energy is lost to solvent.

This hypothesis was explored for the hydroboration of internal disubstituted and trisubstituted alkenes. The applicability of transition state theory and the role of dynamics in determining the selectivity was gauged by determining product ratios in the presence of large excesses of borane and by considering the energetics of the calculated hydroboration reaction path. In all cases the enthalpic barriers for the rate-limiting association step and the formation of products from the intermediate π-complex were small. Isotope effects were determined experimentally and were found to be too small for the conventional mechanism to be the predominate pathway.

When the hydroboration reaction of propene with BH_2Cl or $BHCl_2$ was explored through a series of experimental and theoretical studies, we observed that the regioselectivity was lower than that predicted from transition state theory. However, the calculated pathways indicated that energy barriers for product formation were too large for this reaction to be considered a "hot" reaction. The regioselectivity discrepancy was attributed to the chloroboranes undergoing equilibration with selective reaction of the most highly reactive forms of the borane.

DEDICATION

This dissertation is dedicated to Fransico M. Franco-Torres. A great friend that became my family away from home as soon as I arrived to College Station and whose sacrifices in life inspired positive decisions in mine. To whom I am greatly indebted.

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CHAPTER I

INTRODUCTION

Organoboranes are among the most interesting and important organometallic compounds, and they are particularly valuable as intermediates in organic synthesis due to a variety of chemical transformations that afford organic products with precise structural control. Organoboranes have a number of attractive characteristics that make them useful as chemical reagents. They are relatively unreactive and can coexist with a wide variety of functional groups. The boron-carbon bond has a low polarity and is strong (although easily oxidized) and stable. Organoboranes retain their stereochemical configuration under harsh conditions. Finally, boron can bond with up to three different organic groups, and unsymmetrical organoborane compounds usually redistribute very slowly. These properties allow the design and precise control of more complex organic structures.

There are a number of methods to generate organoborane compounds, each with their own advantages and drawbacks. Transmetallation reactions, where boron exchanges a halide, alkoxide, amine, or thiolate group with an organic group bound to a metal, have been common. These reactions can include many different type of organic groups such as alkyl, aryl, alkenyl, or alkynyl. A second method for generating organoboranes is allylboration. Allyl groups bind to boron and undergo an allylic rearrangement when boron has vacant orbitals. These allylboranes can then react with

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This dissertation follows the style of the *Journal of the American Chemical Society.*

some alkenes and alkynes to form allylated products containing new boron-carbon bonds. The range of successful reactions is somewhat limited, but if the desired product can be formed then this is a convenient process. Diboronation uses diboron compounds (B_2X_4, X=Cl or F) compounds to react with alkenes and alkynes to yield diboryl compounds. Syn addition of the boryl groups is normally observed. Unfortunately, B_2X_4 compounds are not readily available. A Friedel-Crafts type reaction of trihalogenoboranes (with the exception of BF_3) with aromatic molecules can be used to synthesize arylborane compounds. However, the most important synthetic reactions to prepare organoboranes is the hydroboration reaction, where an olefin reacts with borane to form an alkylborane compound, as first reported by Brown in 1956.[1]

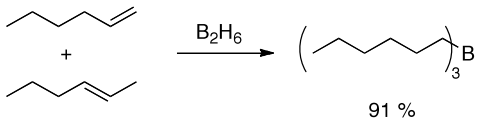
Some observations that foreshadowed the reaction of unsaturated carbon-carbon bonds with boron compounds were first reported by Hurd in 1948.[2] Hurd reacted diborane with a series of olefins (in a large excess) at high temperatures and found that saturation of the double bond occurred to form trialkylboranes. In the presence of a benzene ring phenyl boron compounds formed, while the reaction of diboranes with paraffins forms "polymeric reaction products containing boron, carbon, and hydrogen".[2] Hurd assumed that the active agent in the reaction between diborane and hydrocarbons was most likely a BH_3 molecule. Shortly thereafter, Brokaw observed that in the process of reacting 1-butene with $Al(BH_4)_3$, the two substances underwent a slow reaction, even in the absence of O_2.[3] He also observed that no reaction occurred between $Al(BH_4)_3$ and saturated n-butane. The authors believed that $Al(BH_4)_3$ most likely decomposed into BH_3 which was then available to react with the olefin to form trialkylborane. This

agreed with Hurd's assumption that BH_3 was the active reagent. Stone and Emeleus reported similar findings upon exposing styrene to diborane at room temperature.[4] In the process of carrying out studies on the use of diborane as a reducing agent for organic compounds that began a decade earlier,[5] H. C. Brown discovered that the addition of diborane to olefins in ether proceeded "with remarkable ease and speed at room temperature" to form organoboranes.[6] This process was briefly described in a communication written by Brown[7] and would later become what is now known as the hydroboration reaction. Brown was credited and was awarded the Nobel Prize in 1971.

In the newly discovered hydroboration reaction, it was observed that in the presence of ether the reaction proceeded rapidly (over the course of several minutes) and the placement of the boron atom was on the terminal carbon when using a terminal olefin.[8] Brown and Rao also found the reaction to be highly selective; the reaction of a small amount of diborane with 1- and 2- hexene afforded tri-*n*-hexylborane, with a yield of 91% (Scheme 1.1).[8] It was demonstrated that the crude organoborane products could be oxidized with hydrogen peroxide to form 1-pentanol or 1-hexanol. Interestingly, when the organoborane, from 2-pentene, was oxidized, 2- pentanol (63%) and 3-pentanol (37%) formed.[6] The same study revealed that when the crude organoboranes were subjected to high temperatures, isomerization occurred and 1-alkylboranes were formed, leading to the formation of primary alcohols after oxidation. Additionally, Brown demonstrated that the alkylboranes containing shorter alkyl chains could also be displaced by bulkier alkyl groups. Using ether with diborane proved not only to be a fast and convenient method to produce trialkylboranes, but it also proved to be very versatile

and included many types of terminal olefins, trisubstituted olefins, tetrasubstituted olefins, and aryl substituted olefins.[9] It was establish that most reactions formed trialkylboranes, on the other hand; trisubstituted and tetrasubstituted olefins formed di- and mono-alkylboranes, respectively.[9]

Scheme 1.1



Soon after, it was realized that hydroboration provided a straightforward synthetic strategy for the sterospecific hydration of carbon-carbon double bonds. Brown and Zweifel found that hydroboration could be applied toward acetylenes to form cis olefins and transform terminal acetylenes into aldehydes.[10] These authors also demonstrated that the reaction between 1,3-butadiene and diborane yielded 1,4-butanediol (small amounts of 1,3-butandediol also formed) after oxidation with hydrogen peroxide.[11] Similar results were seen for the conversion of 1,5-hexadiene to 1,6-hexadediol as well. When a competitive reaction showed the preferential hydroboration for 1-hexene over 1,3-butadiene, it was concluded that conjugation decreases the reactivity.[11]

Brown and co-workers developed methods for the reduction of different functional groups by adding $AlCl_3$ to a solution of $NaBH_4$ in diglyme and noticed that organoborane compounds formed at room temperature.[1] Olefins that contained reducible functional groups (ethyl cinnamate and ethyl oleate) not only underwent

hydroboration on the double bond, but also underwent the reduction of the ester group as well.[12] The boron addition occurred on the terminal or less substituted carbon atom while the hydrogen atom added to the more substituted carbon. Sodium borohydride in the presence of boron halides as well as aluminum borohydride in ether were found to induce the hydroboration reaction at room temperature to undergo the anti-Markovnikov addition to form organoboranes.[6,12]

Within a few years of the first developments of the hydroboration reaction, the versatility of hydroborations of olefins, dienes, and acetylenes was known, and a number of research groups were already employing the hydroboration reaction in organic synthesis.[13] Though the applicability of the hydroboration reaction was developing quickly, little was known about what influenced the direction of addition of the boron groups to the unsaturated carbon-carbon bonds, i. e., the regioselectivity. Brown and Zweifel studied what affected the product distribution by considering the hydroborating agent (e.g. – $LiBH_4$, $NaBH_4$, and diborane), solvent system (ethyl ether, tetrahydrofuran, or diglyme), and temperature. All boron-reagent and solvent combinations in the hydroboration of styrene resulted in negligible changes in product distribution, with the exception of a slight increase of the α-derivative at higher temperatures.

The boron addition to the α or β carbon is influenced by the structure of the olefin molecule, examples are shown in Figure 1.1. A brief summary of the literature[14] on how the olefin structure, with reaction examples in scheme 1-5, affects the regioselectivity is given in the scheme below. Many different classes of olefins have

been studied and there is a general preference for the boron addition to proceed in an "anti-Markovnikov" fashion.

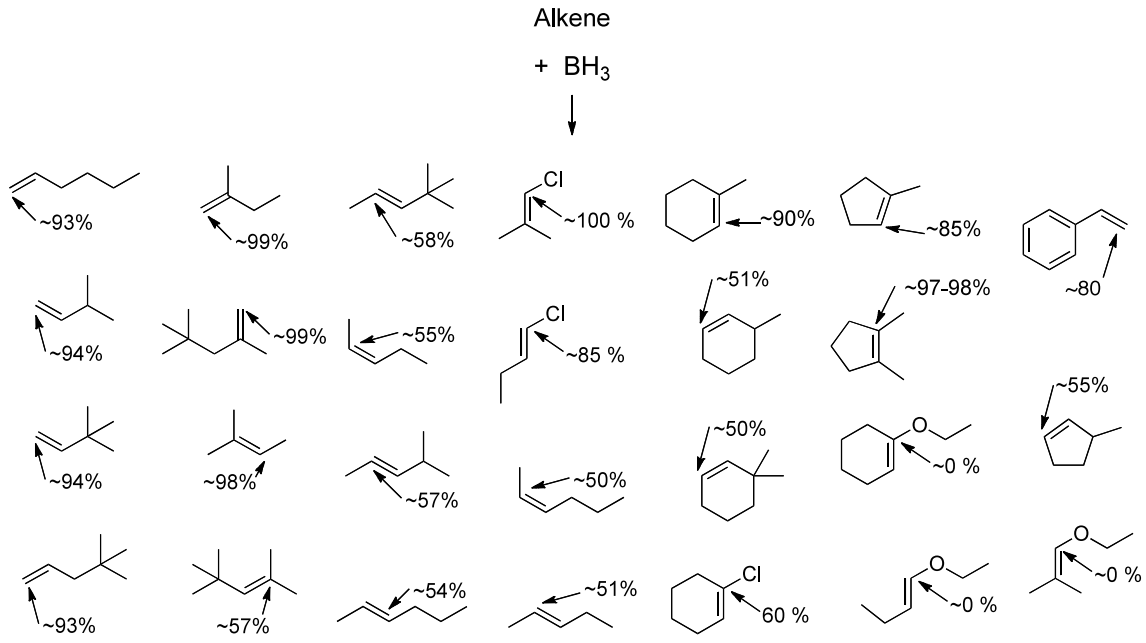
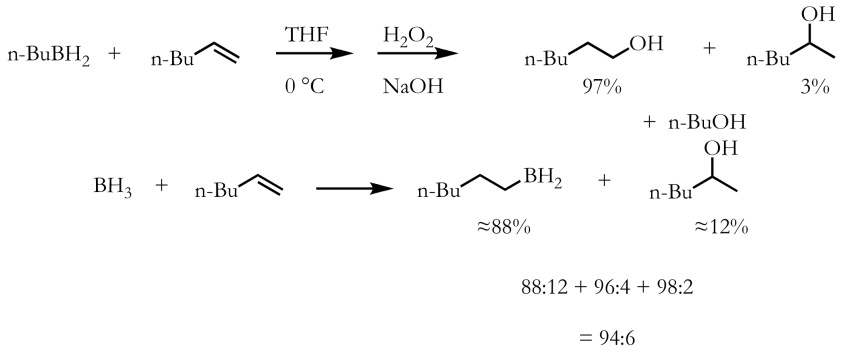


Figure 1.1. Regioselectivity for the hydroboration of various alkenes with BH_3.

In the hydroboration of 1-hexene, 94% of the product formed is 1-hexanol and the remaining 6% is 2-hexanol. This result is complicated because to observed regioselectivity results from hydroboration by BH_3, by alkylboranes, and by dialkylboranes. As shown Scheme 1.3, the hydroboration of 1-hexene with an alkylborane is more selective. Using the observed 1-hexanol/2-hexanol ratio of 97:3 for the reaction of n-butylborane with 1-hexene [15] as a measure of the selectivity of the second and third steps of hydroboration, the regioselectivity for reaction of 1-hexene with BH_3 itself would be ≈88:12. When unhindered, the intermediate alkylboranes are more reactive[16] but they are more regioselective as well.

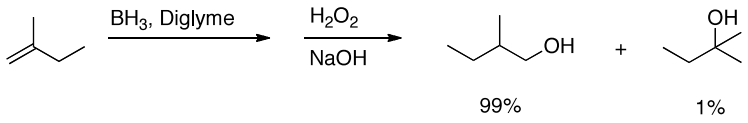
Scheme 1.3



Branching the alkyl chain (such as 3,3-dimethy-1-butene or 4,4-dimethyl-1-pentene) has little effect on the regioselectivity. However, phenyl groups have a significant effect. With styrene, only approximately 80% of the product is the primary alcohol. With allylbenzene, 90% is the primary alcohol.

1,1-Disubstituted olefins show almost complete conversion to the primary alcohol. An example is the hydroboration of 2-methyl-1-butene (Scheme 1.4), which affords 99% 2-methyl-1-butanol and 1% 2-methyl-2-butanol:

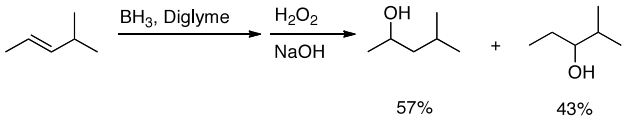
Scheme 1.4



Interestingly, internal disubstituted olefins tend to give nearly a 50:50 product mixture as seen in the hydroboration of 2-hexene or 2-pentene. When the alkyl group is

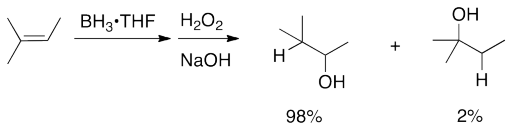
branched, the boron slightly prefers to add to the less substituted carbon atom. For example, the hydroboration of trans-4-methyl-2-pentene (Scheme 1.5) affords 57% and 43% of products where the boron was added on the second and third carbons, respectively.

Scheme 1.5



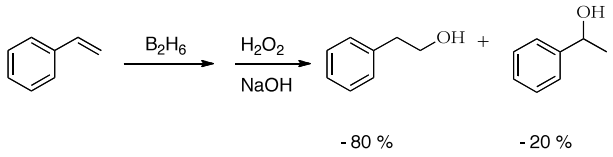
Trisubstituted olefins lead to high selectivity. The hydroboration of 2-methyl-2-butene affords 98% of the secondary alcohol and 2% of the tertiary alcohol as is shown in Scheme 1.6. Only the dialkylborane intermediate is obtained when using trisubstituted alkenes. This reaction will be further discussed in Chapter IV.

Scheme 1.6



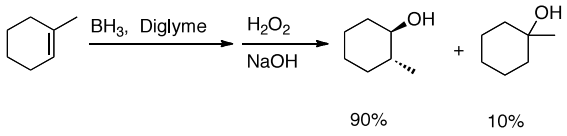
The regioselectivity of the hydroboration of styrene derivatives is affected by electronic effects. The hydroboration of styrene yields 20% of the products form alcohol on the alpha carbon and 80% on the beta carbon as seen in Scheme 1.7. However, when the para-position on the styrene contains a methoxy-, methyl- or chloro- group the resulting alcohol contains 9%, 18%, and 35% of the alpha isomer, respectively.

Scheme 1.7

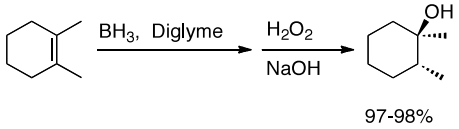


The product distribution arising from cyclic olefins (1-methylcyclopentene, 1-methylcyclohexene, and 1-phenylcyclohexene) was studied as well. It was found that the reaction is stereospecific and the addition to the double bond occurs in an anti-Markovnikov *syn* fashion.[17] As an example (Scheme 1.8), 1-methylcyclohexene was converted to trans-2-methylcyclohexanol. In the case of 1,2-dimethylcyclohexene, shown in Scheme 1.9, the preferred product was the more thermodynamically unstable cis-1,2-dimethycyclohexanol. Similar results were found for 1-methylcyclopentene and 1,2-dimethycyclopentene and in all cases 97-98% of the product consisted of the indicated dominant isomer.

Scheme 1.8



Scheme 1.9



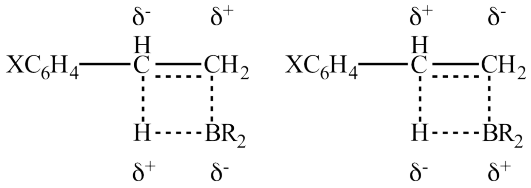
Hydroboration was also studied with rigid bicyclic olefins including norbornene, α-pinene, β -pinene, and camphene. These reactions afford *exo*-norborneol, isopinocampeol, *cis*-myrtanol, and *endo*-camphenol, respectively.[17b] When the hydroboration reaction was applied to 3-alkylcycloalkenes, such as 3-methylcyclopentene, little control over the product distribution was achieved (48% on carbon 2 and 52% on carbon 3). This may partly be attributed to the equatorial position of the methyl group that does not provide much steric influence to the addition of the boron atom. Accordingly, the hydroboration of 3,3-dimethylcyclohexene revealed slightly more control with 40% of the boron addition on carbon 3 and 60% on carbon 2.

The general results that Brown and Zweifel obtained indicate that the electronic effect of the substituents on the olefin as well as their steric effect may play a role in the regioselectivity. However, it should be noted that the hydroborations of 1-butene, 3-methyl-1-butene, t-butylethylene, and neopentylethylene all afford~93% of the anti-Markownikoff product. Perhaps one may expect a more significant difference when considering steric effects.[14] Nonetheless, Brown repeatedly included sterics in explanations of the regioselectivity of hydroborations.

Scheme 1.10

Brown and co-workers proposed that the hydroboration reaction proceeded through a 4-center transition state where the α- and β- carbons have a partial positive and negative charge and the hydrogen and boron posses a partial negative and positive charge, respectively (Scheme 1.10).[14,17b] In the case of styrene it may be reasonable to assume that the phenyl group may stabilize a negative charge on α- carbon and showed an enhanced selectivity for the boron addition to occur on that carbon. This theory was studied by hydroborating styrene with a number of different substituents, with various electron-withdrawing capabilities, on the ortho, meta, and para position under standard conditions (diglyme, 20 °C).[18] The product distribution of the addition of boron on the α-carbon for styrene consisted of 19% while the respective distribution for the substituted derivatives of styrene of *o-, p-, m-* methoxystyrene was 14%, 7%, and no effect, *o-, p-, m-* chlorostyrene was 26%, 30%, and 27%, *o-, p-, m-* trifluoromethylstyrene was 38%, 32%, and 34%, and *m*-nitrostyrene was 37%. The product selectivity agrees reasonably well with the σ^+ plot and indicates that the reaction proceeds through an electrophilic attack by the boron. It should be pointed out that the effects of the different substituents on styrene only varied slightly.

Scheme 1.11



From their various observations, Brown and Zweifel concluded that the four-centered transition state was impacted by steric and electronic factors (Scheme 1.11).[14,17a] A Hammett correlation of log (terminal/internal) ratios from the hydroboration of substituted styrenes in diglyme worked best with σ^+ and exhibited a ρ of -0.7, supporting the role of electronic effects.[18]

Klein evaluated the hydroboration of styrene derivatives in THF by a combination of absolute kinetics under pseudo-first-order conditions and regiochemical observations. Hammett plots for the boron attacking the alpha position of the *m*-, and *p*-substituted styrene and at the *m*- substituted for the beta position produced linear correlations with ρ = 0.5, 1.2, and -0.5 respectively.[19] Klein made the critical observation that the effect of substituents on the regioselectivity was much greater than their effect on the absolute rates, the latter varying little with substituents. The led Klein to write in 1966:

> An attractive although not compelling explanation for the much higher positional than intermolecular selectivity is the formation, during the reaction, of an intermediate π-complex between borane and the olefin. …The formation of the complex would then be insensitive to the structure of the olefin and would proceed with most of them with comparable rates. This complex rearranges by way of the transition states postulated by Brown to the products. The differences between the energies of the transition states leading to the isomers are larger than the differences in the

activation energies for complex formation between borane and various olefins.

Klein's proposal that hydroboration occurs by the rate-limiting formation of a π-complex followed by regioselectivity-determining steps was largely ignored, though it is a conclusion of this dissertation that except for the role of dynamic effects, Klein (alone) had the correct mechanism.

Kinetic studies with substituted boranes are simpler than those with BH_3 and have been carried out extensively. The hydroboration of alkenes with disiamylborane or monochloroborane as the hydroborating agent showed that the reactions were first order in the borane and the olefin.[20] The log (terminal/internal) product ratio correlated with σ and showed ρ = -0.65. The hydrogen-deuterium isotope effect for the reaction of styrene with monochloroborane-THF was 1.90.[20b]

The earliest studies of hydroboration focused on unsaturated hydrocarbons and little attention was paid to how functional groups affected the regioselectivity of the boron addition. Later studies looked at alkyl halides and ethers. When vinyl halides are hydroborated the boron atom preferentially attaches to the carbon with the halogen (α-carbon). This leads to alpha-haloorganoboranes-carbenes intermediates in a rearrangement that ultimately replaces the halogen with a hydrogen.[21] Beta-haloorganoboranes undergo a rapid elimination of boron-halogen to form an olefin.[21] In the case of allyl chlorides, it was shown that the electronegative substituents direct the addition of boron toward the beta-carbon and generally give a product distribution of 82:18. When allyl chloride or allyl tosylate is used, 40% and 45%, respectively, of the

product have the boron placed on the secondary carbon.[22] The hydroboration of crotyl derivatives shows a preference toward the boron adding to the beta-carbon position with electronegative substituents enhancing this directing effect further. For example, the addition of boron on the beta-carbon was 100% for crotyl chloride while only 84% for crotyl ethyl ether.[23] In the hydroboration of of vinyl derivatives, the regioselectivity depends on the substituent. Interestingly, chloro and acetoxy derivatives of vinyl give products with boron on both the alpha and beta position.[24]

The structure of the hydroborating agent has a large effect on the regioselectivity. For instance, bis(3-methyl-2-butyl)borane (disiamylborane) provides "steric control" of the hydroboration reaction and more selective formation of the less hindered alcohol. In the hydroboration of 1-hexene with disiamylborane, the regioselectivity is increased to 99%.[25] Unlike diborane[26], disiamylborane is highly sensitive to the structure of the olefin; 1-alkenes react 50 times faster than *cis*-2-alkenes, and 300 times faster than trans isomers. This allows selective reactions of molecules containing multiple unsaturated centers.

Many alkyl-substituted boranes show increased regioselectivity due to steric or electronic factors. As mentioned previously, the hydroboration of styrene with diborane affords 80% of the primary alcohol, but the sterically hindered thexylborane affords 96% of the primary alcohol.[27] Thexylborane, disiamylborane, and diisopinocamphenylborane led to 98.9%, 99.0%, and 100%, respectively, formation of 3-cyclopentenol in their hydroborations of cyclopentadiene.[28]

Organoboranes with thiolate ligands were investigated for their reactivity and selectivity. In one of the first examples, Schegoleva and Belyavskaya reacted propylene with $C_2H_5SBH_2BH(SC_2H_5)_2$ to form $(C_3H_7)_2BSC_2H_5$ (25%) and tetraethylthiodiborane (33%).[29] Mikhailov produced mixtures of $C_4H_9SBR_2$, BR_3, and $(n\text{-}C_4H_9S)_2BH$ through the reaction of ethylene, propylene, and 1-hexene with $(C_4H_9SBH_2)_x$ in diethyl ether.[29c] However, it is probable that the harsh reaction conditions encourage disproportionation. Pasto and co-workers produced phenylthioborane with thiophenol and borane in tetrahydrofuran (THF). These conditions caused cleavage of the THF solvent which limited the amount of phenylthioborane formed.[30] The selectivity of the hydroboration reaction between phenylthioborane and styrene (2-phenylethanol:1-phenylethanol; 91:9) was very different than what has been previously reported for styrene with borane in THF (81:19).[30] Brown and co-workers later prepared monochloroborane-methyl sulfide and dichloroborane-methyl sulfide as highly stable and regiospecific hydroboration agents.[26] In most cases, the alcohol generated from the oxidation of the final organoborane product almost exclusively yielded the primary alcohol such as 1-hexanol (99.2%), 2-phenylethanol (93%), 2-methyl-1-butanol (99.9%), exo-2-norbornanol (99.5%), 3-methyl-2-butanol (99.5%), trans-2-methylcyclopentanol (99.5%), and 2-phenyl-1-propanol (99.9%).[31] Brown then demonstrated that dibromoborane-methyl sulfide is a highly active hydroborating agent that did not require a Lewis acid (such as BCl_3).[32] In this case, the product distribution was 1-hexanol (99.6%), 2-phenylethanol (96%), 2-methyl-1-pentanol (98%), 2-pentanol (67%), 3-methyl-2-butanol (93%), and trans-2-methylcyclopentanol (98%).[32]

Initial experiments performed by Pasto and Zweifel indicated that the hydroboration of olefins with monochloroborane in THF was slow compared to BH_3-THF.[33] If the hydroboration reaction happens by an electrophilic attack on the olefin double bond by the boron,then it should be expected that the chloroboranes would exhibit a high rate of reaction. The slow rate of reaction was attributed to the strong complexing interaction between the chloroboranes and THF, diminishing the electrophilicity.[33] This hypothesis was supported by comparing the chemical shifts (^{1}H-NMR) with borane in THF and monochloroborane in THF.[33a] Brown showed that if a less basic solvent, such as diethyl ether or diglyme, was used the rate of reaction between the olefin and monochloroborane increased due to the weakened complexing interaction with the solvent.[34] Dioxane proved useful as a less environmentally harsh solvent that was capable of producing moderately fast reaction rates.[35]

It was found that alkylchloroboranes could greatly improve the directing effect of the hydroboration reaction and even obtain yields >99.5%. The use of monochloroborane showed an improvement directing the addition of the boron atom to the least substituted carbon as seen with the hydroboration of 1-hexene with monochloroborane in THF. The experiment resulted in a slight increase in the anti-Markownikoff product (96:4; compared to 94:6 using BH_3-THF). Increased selectivity was also seen in the case of styrene where the product mixture contained 2-phenylethanol (89.8%) and 1-phenylethanol (10.2%).[33a] The use of diethyl ether proved to be a powerful directing agent and selectivities toward the formation of the alcohol on the terminal carbon, after oxidation with alkaline hydrogen peroxide, achieved almost

100% in some cases.[36] The use of dioxane as a solvent with monochloroborane showed regioselectivities similar to diethyl ether. The hydroboration of this adduct with unhindered or slightly hindered olefins occurs within 30 minutes to several hours, respectively; while tetrasubstituted olefins form monoalkylchloroboranes rapidly and further hydroboration proceeds slowly.

Hydroborations using dichloroborane were studied as well. The reaction was found to proceed very slowly in THF and diethyl ether compared to monochloroborane, further confirming that interaction with THF influences the rate of reaction.[33,37] In all reactions reported, the main product resulted from boron addition to the least substituted carbon atom, except in one early study it was reported that dichloroborane showed preferential formation of the Markovnikov addition product.[38] Using a stronger Lewis acid, such as BCl_3, helped to remove the complexed ether and allowed the reaction to occur at a faster rate.[38] In 2001, Brown showed that $BHCl_2$-dioxane preferred the hydroboration of 2-substituted terminal olefins in the presence of simple terminal olefins. Dichloroborane in monoglyme or β-chloroethyl ether exhibited high reactivity at room temperature toward unhindered olefins, but hindered olefins required higher temperatures or the addition of one equivalent of BCl_3.

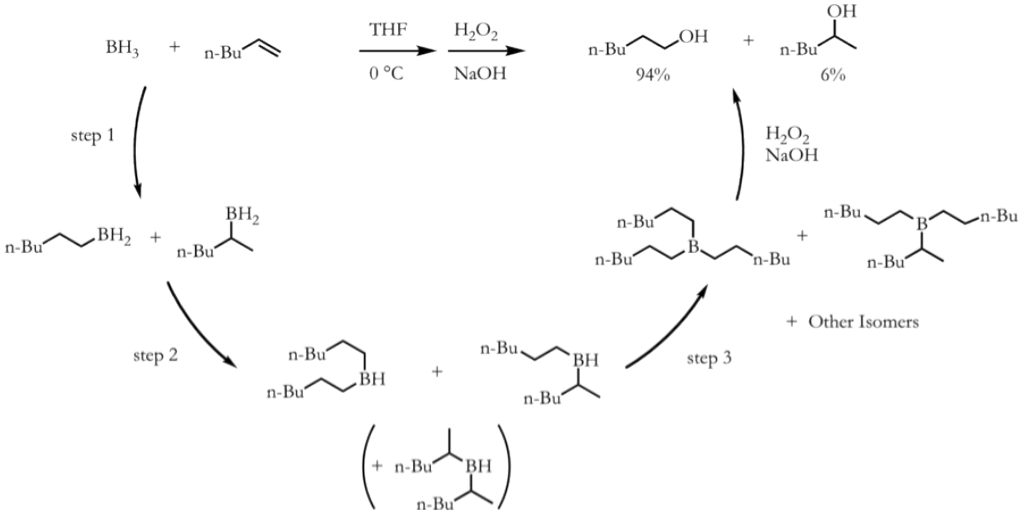
Pasto investigated the mechanism of the hydroboration reaction in kinetic studies. Pasto found that the reaction of tetramethylethylene with borane in tetrahydrofuran was first order in the borane and the tetramethylethelene as well. The activation energy for the same reaction was found to be 9.2 ± 0.4 kcal/mol and the entropy of activation was -27 ± 1 eu. Pasto determined an intermolecular hydrogen-

deuterium kinetic isotope of 1.18 from the absolute kinetics.[39] These results in combination with Pasto's previous NMR experiments with borane in THF[33a] meant to him that a BH_3-THF complex is formed. In addition, when comparing the activation energy on the gas phase reaction of ethylene in borane (2 ± 3 kcal/mol)[40] shows that the solvent does play an important role in the reaction. Also considering the predicted entropy of activation for the gas phase reaction of borane with tetramethylethylene is ~-29 eu[40], which fairly agrees well with the experimental values. These results were taken as suggesting that the BH_3-THF complex undergoes a direct reaction with the alkene as opposed to a dissociation of the complex to afford intermediate free borane. From ^{10}B-^{11}B and intramolecular hydrogen-tritium isotope effects, Pasto concluded that Brown's hypothesis of a four-centered transition state[14,17] was correct. In contrast, Brown's work consistently supported a mechanism in which the BH_3-Lewis base complex dissociates to free BH_3 before undergoing the hydroboration reaction.[7]

Pasto also investigated the reaction kinetics for the formation of di- and trialkylboranes by the hydroboration in THF, the kinetics for alkylborane-borane redistribution reactions, and the equilibrium constants for the alkylborane monomer dimer equilibria (Scheme **1.12**).[16] Pasto's experimental findings indicated that the formation of dialkylborane proceeded through consecutive addition reaction because the rate of reaction was much faster versus a disproportionation pathway.[16] It was also explained that the reaction rate of the hydroboration involving mono- and disubstituted alkylboranes as compared with BH_3 with alkenes in THF was much higher due to the increase in complexation strength.[16] The increase in substituents on the borane caused a

decrease in stability in the following order, $BH_3 \cdot THF > RBH_2 \cdot THF > R_2BH \cdot THF$, thereby increasing the reactivity. Based on these results, the hydroboration mechanism is explained in every organic chemistry textbook.

Scheme 1.12



By the late 1970's and early 1980's a significant amount of work had already been done on studying what factors influence the direction of addition of the boron atom to the alkene's double bond, applying computational techniques to help explain the reaction mechanism and the experimental selectivity. In 1967, Streitwieser reported an alternate mechanism that suggested the intermediate formed a triangular π-complex and formed a three-center transition state.[41] Similarly, Dasgupta used the CNDO/2 method to calculate the energies of the optimized 3-center and 4-center complexes. He found the 3-center structure to be slightly more stable and considered it as the transition state.[2] MNDO studies by Dewar and Mckee[42] of the hydroboration of a wide variety of alkenes

and alkynes agreed with this prediction. The results supported the theory that steric effects influence the regioselectivity. Interestingly, they predicted that the hydroboration vinyl chloride and vinyl fluoride with borane would produce the Markovnikov and anti-Markovnikov products, respectively.[42] Morokuma[43] and Houk[44] used ab initio methods, while Lipscomb[45] used PRDDO methods to study the transition state of the hydroboration reaction, and they all favored Brown's four-centered transition state π-complex. It was shown that the formation of the π-complex before the development of the transition state was exothermic and downhill by 5.6-11.7 kcal/mol from the reactants.[43,45-46] An interesting result was also discovered by Lipscomb that showed that when configuration interaction calculations on close-shell wave functions were used the correlation energy actually stabilized the transition state of the reactants and products and that no activation barrier was found for the zero-order configuration interaction level.[45] These result agree with Clark who also found a zero activation energy for the hydroboration reaction using STO-3G and 4-31G levels, but did not study the effects of configuration interaction.[47] Houk predicted that the transition structure of diborane with ethylene was a borane ethylene complex with a nearly dissociated borane.[44e] However, even though the π-complex is predicted to be more stable at various levels of theory it disappears when correlation energy corrections are included.[44e] For instance, the energy difference between the transition state and the complex was 13.9 kcal/mol (3-21G), 9.1 kcal/mol (6-31G), and 5.7 kcal/mol (MP2/3-21G) which suggest that the transition structure does disappear as well as suggesting that there is also no activation energy

(Figure **1.2**). He also showed that electronic and steric affects govern the regioselectivity of the product[44e]

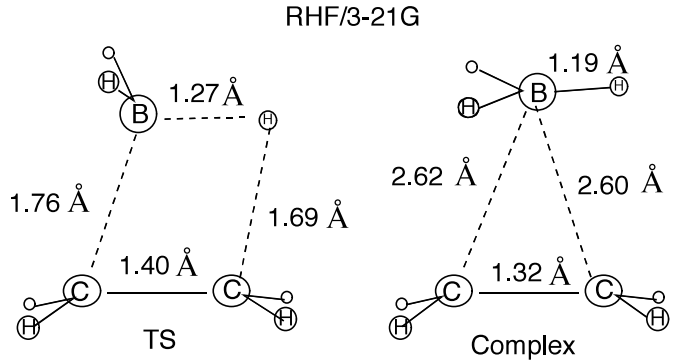


Figure 1.2. Transition state and π-complex structures located by Houk for the hydroboration of ethylene with BH_3.

The studies above assumed the applicability of transition state theory (TST). TST has been a highly successful and reliable basis for understanding reaction mechanisms, and it was only logical to apply TST to hydroboration.

When assuming TST toward the hydroboration reaction, as was done by the authors above, it is important to understand that in this theory the barrier for product formation is used to explain the rate of a reaction. Kinetic selectivity is then decided by the difference in barriers for formation of alternative products, though some exceptions to this rule are known.[48] What makes the computational results of Lipscomb interesting is that he observed the absence of an enthalpic barrier. The result Houk found suggests that a transition structure actually disappeared with higher levels of calculations.

In some cases TST may not be an appropriate method to use for modeling reaction reactivity and selectivity. Other theories such as, dynamic effects, have prove

to be more accurate computational models to follow due to its inclusion of entropic barriers. Transition state theory is a model for reactivity that can fail, and we will refer to such failures as 'dynamic effects'. The origin of this term is that when transition state theory fails, one must fall back on the detailed consideration of the motions and momenta of atoms. This term is unfortunately confusing because "dynamics" is often used as a synonym for kinetics, and "dynamic effects" has been used to refer to the effects of conformational equilibria, particularly in enzymes. The consideration of dynamic effects is essential for the understanding of the mechanism in a diversity of reactions.[49]

A consideration of the potential energy surface in Figure **1.3** shows that different products may come from the same transition state by proceeding through two product wells without an energy barrier. In this case, the formation of the two products is intertwined but the selectivity is obviously not associable with two transition state energies. It is then necessary to consider dynamics to predict the branching of products.[50] Surfaces resembling this portrayal are typically associated with symmetry breaking and have been explored theoretically for many simple reactions. As will be seen, this is not the only circumstance in which dynamics is important, but it is a readily understandable example.

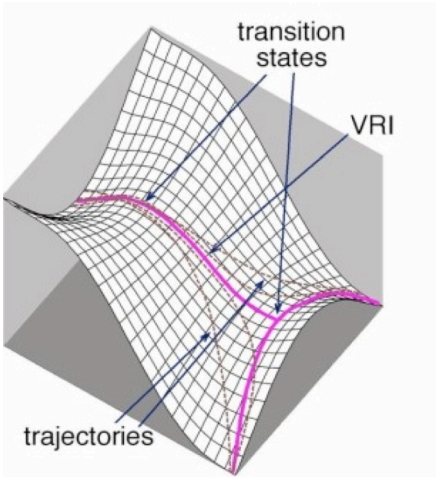


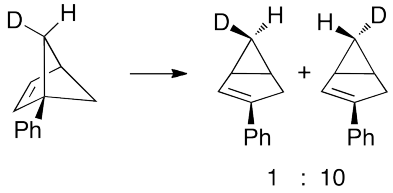
Figure 1.3. A symmetrical potential energy surface in which the trajectories can split into two products at the second transition state.

Calculating a large array of individual trajectories with a variety of initial conditions provides a prediction of the ratio of the products. The results from such trajectory calculations can then be easily judged against the experimental ratio of products and facilitate the development of a mechanistic model.

Carpenter and co-workers first began to consider the dynamic effect in 1984 when they studied the temperature dependence of the stereoselectivity of the rearrangement of bicyclo[2.1.1]hexane-5-d and its phenyl derivatives.[51] It was found that temperature dependence was associated with the parent compound and suggested a parallel reaction pathway with different activation energies may be present while the phenyl derivatives are temperature independent and prefer retention of configuration (Scheme **1.13**).[51] A product ratio of 9:1 and 5.9:1 ratio was obtained with the reaction of 1- and 2-phenylbicyclo[2.1.1]hex-2-enes-5-d and trans-2-methyl-1-(trans-2-phenylethyenl)cyclopropane, respectively, with similar activation enthalpies.

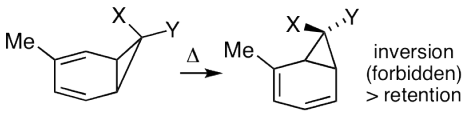
Interestingly, these results did not seem to completely concur with the major theories such as RRKM theory, TST, and variational transition state theory, but appeared that dynamic effects were directly involved.[52]

Scheme 1.13



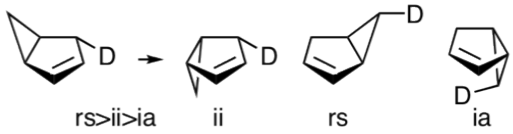
A year later, it was shown that trajectories on a potential energy surface take the reactants through an intermediate and to the product in a straight-line path.[49b] It was also found that nonstatistical dynamical effects may be involved in the thermal deazeitization of 2,3-diazabicyclo[2.2.1]hep-2-ene and that the transition structure corresponded to "synchronous C-N cleavage" with an alternative mechanism involving the stepwise C-N bond scission (7 kcal/mol higher).[53] Previous studies predicted the reaction to proceed through the later mechanism mentioned earlier. Carpenter later found that branching from the acetone radical cation occurred in an unusually deep potential well showing nonstatistical dynamics.[54] When trajectories originating from the top of the transition state were run the reaction rates were enhanced when compared to starting at the acetone radical cation minimum. [54] In the study of bicyclo[n.1.0]polyenes, it was determined that the ring walk rearrangements were pericyclic with a preference for the inversion of configuration at the migrating carbon[55]

Scheme 1.14



Doubleday and co-workers applied quasiclassical direct dynamics simulations to the degenerate rearrangement of bicyclo[3.1.0]hex-2-ene. They found that a short-lived diradical intermediate is formed and that the product ratio depends on the lifetime of the intermediate. The short intermediate lifetime is a consequence of the potential energy surface's relatively flat potential energy profile. Therefore, a significant amount of trajectories show how momentum was gained by entering high potential energy surface regions and become.[56] The flat surface found here suggests that something else might be happening when there is no enthalpic barrier found in hydroboration.

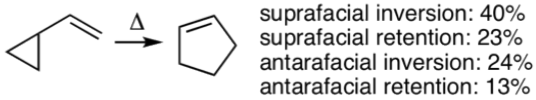
Scheme 1.15



In a separate study, direct dynamics was used to evaluate the stereomutation of cyclopropane and whether if undergoes a concerted double rotation[57] or a competitive concerted single and double rotation.[58] Doubleday and co-workers found that mechanism may undergo a concerted and nonconcerted process in which nonstatistical effects are overriding. The trajectory results are not strongly dependent on the potential energy surface.[57] It was also shown that TST theory predicts that trimethylenes formed by disrotation reclosed by conrotation. The dynamic model predicts direct trajectories

across the potential energy surface overcome a higher energy barrier to exit by disrotation. This results indicate that dynamic matching between entrance and exit entrances outweigh barrier heights and the dependence of details about the surface are not strong.[58a] In another example where dynamic effects proved to be a useful method was in the elucidation of the stereochemistry of the vinylcyclopropane-cyclopentene rearrangement (Scheme **1.16**). For this rearrangement, previous TST calculations showed that there was no local minimum in the biradical region of the potential energy surface, but instead was four broad paths within 2-3 kcal/mol within each other.[59] Unfortunately, under these conditions TST cannot predict product ratios when two or more paths are mediated from a single transition state. Quassiclassical trajectories, run on a modified AM1 potential parameterized to fit ab initio calculations, found that the rearrangement consisted of four competing reactions in competition with C_2-C_3 torsional motion.[60] These results of the trajectory studies accurately matched the experimental product ratios. The product ratio was found not to be dependent on temperature. For trajectory times under 400 fs the product ratio was dependent on time, and above 400 fs the product ratio was statistical.[61] These results indicate that nonstatistical dynamics were involved and the mechanism did not consist of a statistical intermediate.

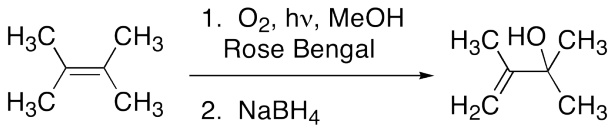
Scheme 1.16



In addition to the work of Carpenter and Doubleday, many examples where it was essential to consider dynamic effects to explain basic chemical observations have

been recognized by the Singleton group.[48,50,62] Singleton and co-workers have studied in detail the mechanism for the ene reaction of singlet oxygen with simple alkenes. As part of this work, intermolecular KIEs were determined for the reaction of singlet oxygen with 2,4-dimethyl-3-isopropyl-2-pentene and intramolecular KIEs were attained for the reaction with tetramethylethylene (Scheme **1.17**). As a consequence of the experimental KIE found, that there was no correlation for the KIEs obtained, the reaction mechanism was proposed to proceed via a two-step mechanism. Nonetheless, no intermediate was isolated or predicted to be at minimum energy according in their experimental and theoretical attempts. The reaction was proposed to involve a bifurcating energy hypersurface, in which there is an early transition state and that singlet oxygen chooses which olefinic carbon attach to when it has reached the valley ridge inflection point. In this system, symmetry breaking step justifies the intramolecular KIE.

Scheme 1.17



Now we intend to study the mechanism of the commonly used hydroboration reactions of various types of alkenes, identify, and understand dynamic effects in these reactions, and compile observations that differ from those expected if TST is accurately applied. Here we examined the mechanism for hydroboration in a series of reactions from an experimental and theoretical approach. A main focus of these studies is the accurate accounting for the regioselectivity, which may differ from that predicted by TST.

CHAPTER II

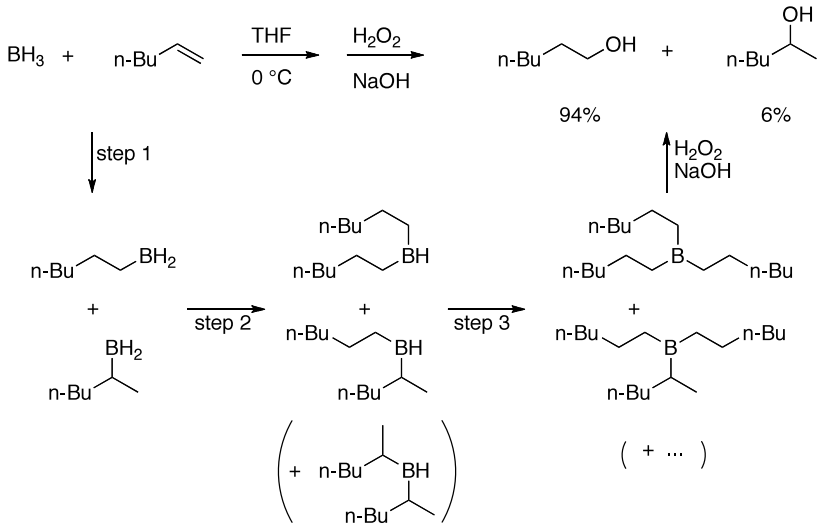
DYNAMICS AND THE FAILURE OF TRANSITION STATE THEORY IN THE HYDROBORATION OF TERMINAL ALKENES WITH BH_3

The hydroboration of simple alkenes with BH_3 preferentially occurs in an "anti-Markovnikov"[14] fashion. The standard explanation for this preference in the literature,[42,44e,63] reproduced in some form in all general textbooks of organic chemistry, is that the selectivity arises from a greater stability for the anti-Markovnikov transition state over the Markovnikov transition state. This explanation presupposes the applicability of the transition state theory *model* for reactivity and selectivity. The work described here finds that transition state theory cannot account for the regioselectivity of the hydroboration of terminal alkenes with BH_3. Instead, a consideration of dynamic trajectories allows understanding of the selectivity.

The addition of BH_3 to terminal alkenes is only moderately regioselective. With simple terminal alkenes such as 1-hexene, the ratio of primary to secondary alcohol products after hydroboration with BH_3 at 0-25 °C followed by oxidation is approximately 94:6.[14,30,64] This ratio as it has been observed is a composite of the regioselectivity in three separate steps – hydroboration by BH_3, hydroboration by RBH_2, and hydroboration by R_2BH (Scheme 2.1). When unhindered, the intermediate alkylboranes are more reactive,[16] but they are more regioselective as well, so the initial reaction of BH_3 is less selective than the composite ratio. Using the observed 1-

hexanol/2-hexanol ratio of 97:3 for the reaction of n-butylborane with 1-hexene[15] as a measure of the selectivity of the second and third steps of hydroboration, the regioselectivity for reaction of 1-hexene with BH_3 itself would be ≈88:12.

Scheme 2.1



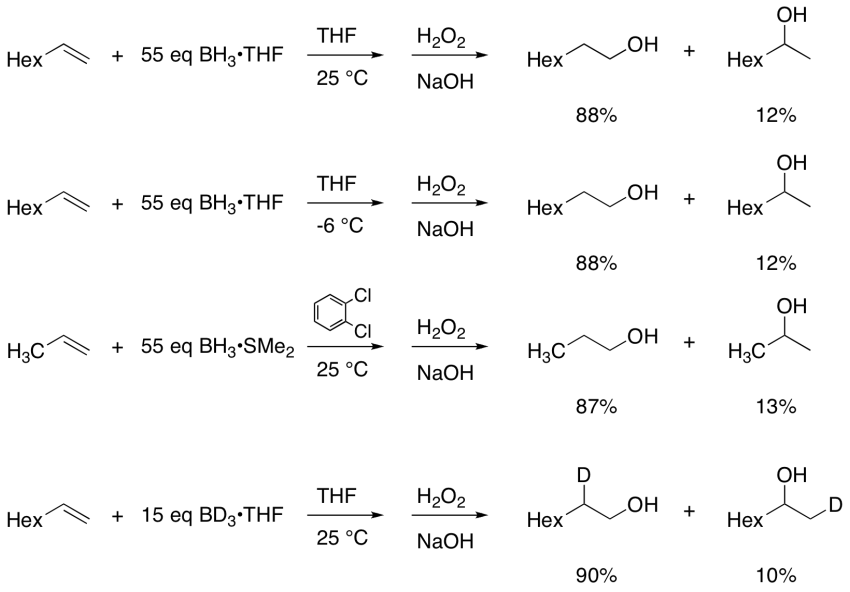
The 88:12 ratio is an estimate of the regioselectivity, and we sought to determine this regioselectivity directly. Our strategy was to use larges excesses of BH_3 to minimize the contribution of hydroboration by alkyl- and dialkylboranes to the observed regioselectivity. Our initial studies examined the hydroboration of 1-octene with BH_3 in THF. The excess of BH_3•THF employed was increased in increments, measuring the ratio of 1-octanol to 2-octanol after an oxidative workup in each case by GC. This approach encountered problems, as the excess of BH_3•THF employed grew larger, particularly when the excess exceeded 55 equivalents. A particular issue was that small

amounts of impurities in the BH_3•THF, possibly arising from THF decomposition, interfered with the analysis.

To an effort to avoid the impact of interfering impurities, we studied the hydroboration of propene with BH_3•THF. However, the GC analysis of 1-propanol to 2-propanol in a mixture of water and THF proved challenging. A concern was that selective loss of the minor regioisomer could occur during purification, so the experimental procedure was designed to obtain the ratio of products with minimal manipulation of the sample. An attempt was made to improve the resolution of the GC peaks by using a MXT-WAX capillary column (30 m x 0.25 mm). This analysis still failed to completely resolve the THF and the 2-propanol. The analysis could be successfully carried out when the solvent was changed to *o*-dichlorobenzene as long as the excess of borane employed was low, but the analysis again failed when using large excesses of borane due to the presence of small amounts of impurities.

Another attempt to determine the hydroboration regiochemistry employed deuterated-borane in THF. It was envisioned that this would allow the direct observation of the regioselectivity in the oxidized reaction mixture by ^2H NMR. This method was a success but was limited in that a very large amount of BD_3•THF is needed, and this was not practical in terms of cost.

Scheme 2.2

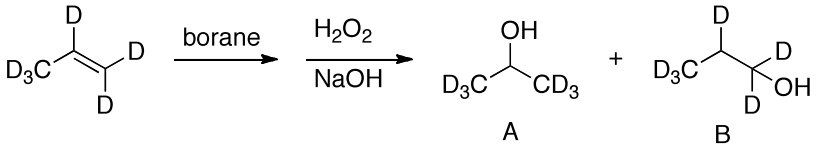


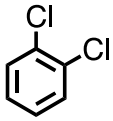
The ultimate economical solution to the problem of determining the hydroboration regiochemistry was to use deuterated alkene. It was found that the hydroboration of propene-d_6 could be carried out with a large excess of BH_3•THF while allowing the direct analysis of the reaction's crude mixture after oxidation by ^2H NMR. This procedure allowed the exploration of various reaction conditions, including varying solvents, temperatures, and borane sources (Table **2.1**).

We considered the possibility that the experimentally observed product ratios were being affected by an isomerization equilibrating the products. Such isomerization might be detectable in a couple of ways. First, the isomerization could lead to an observable change in the product ratio versus time as the reaction approaches its thermodynamically favored product ratio. A problem with this possibility is that the equilibrium product mixture might be obtained very rapidly, in which case the ratio of

products would not subsequently change. A second way to detect isomerization takes advantage of the deuterium labeling in the propene, as equilibration of the distribution of H and D should occur if isomerization is taking place.

Table 2.1. Hydroboration reactions of propene-d_6 with borane.



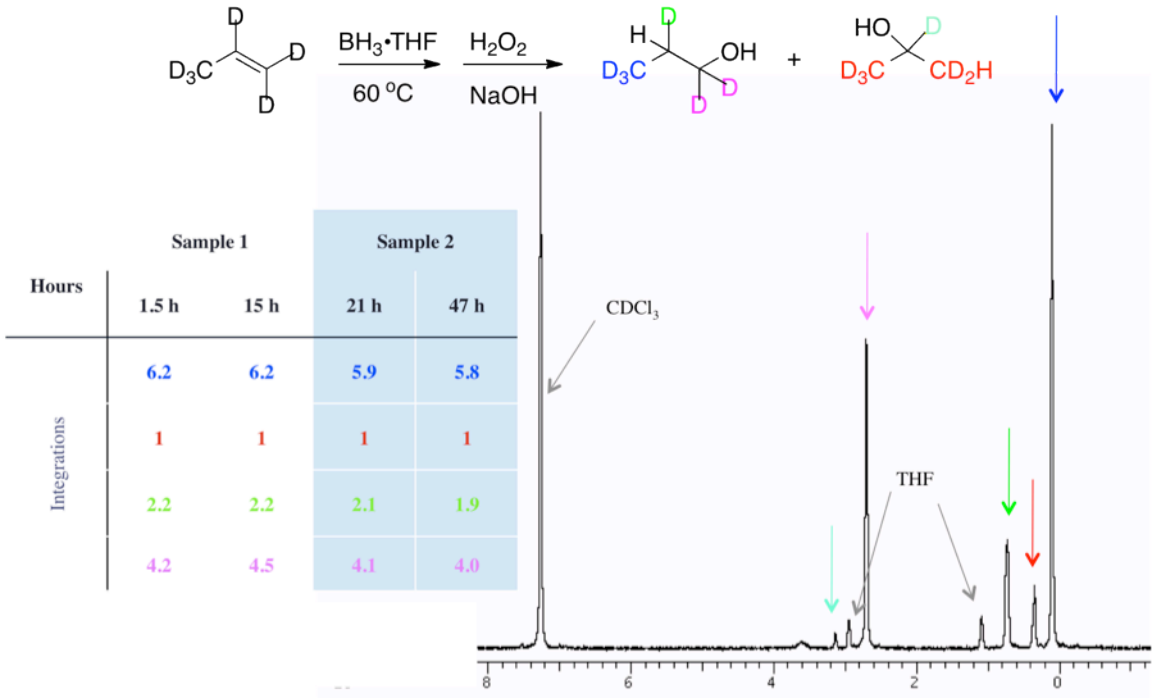
Borane	Solvent	Temp. °C	equivalents of borane	% of A	% of B
BH_3	THF	21	44	7.5	92.5
BH_3	THF	21	100	10.0	90.0
BH_3	THF	70	37	8.6	91.4
BH_3	THF	- 6	37	6.9	93.1
BH_3	THF	21	0.3	4.0	96.0
$BH_3.SMe_2$	none	21	44	5.6	94.4
$BH_3.SMe_2$	diglyme	21	44	5.8	94.2
$BH_3.SMe_2$		21	44	5.5	94.5

To address this issue, we studied the hydroboration of propene-d_6 at 60 °C with 100 equiv of BH_3•THF under conditions that would maximize the amount of isomerization, that is, at 60 °C and employing much longer reaction times than employed for the reactions determining the regioselectivity. As before, we used direct ^2H NMR

analysis of peaks corresponding protons for 1-propanol. If there were no isomerization taking place, the ratio of the deuteriums in the C-1, C-2 and C-3 positions (the CD_2, CHD, and CD_3 positions, located at 2.7, 0.75, and 0.11 ppm versus $CDCl_3$ at 7.25) should be 2 : 1 : 3, respectively. If full equilibration takes place, then the ratio should approach 2 : 2 : 3, respectively. In order to monitor the product ratios we will also integrated the peak corresponding to the chemically equivalent CHD_2 and CD_3 of the minor isomer, which is observed at 0.35 ppm in these samples. The peak for the minor isomer arising from the methine (CDOH) that resonates at ~3.15 ppm was not monitored; this integration was not reliable due to its small size and incomplete resolution.

Figure **2.1** contains a color coded NMR in relation to the product and the integrations for 1.5, 15, 21 and 47 hours, are display in each color as well in the table to the left. The 1.5 and 15 hours belong to the same reaction, 21 and 47 hours belong to another sample. If isotopic equilibration were taking place in the 1-propanol, the integration for the C-2 methylene peak (green arrow) should grow relative to the C-1 methylene and C-3 methyl peaks. It does not. This strongly supports the conclusion that intramolecular isomerization or isotopic equilibration does not occur to any significant extent on the much shorter time scale of the reactions in which the regiochemisry was measured. It seems possible from the data that the regioselectivity, as judged by the methyl group peak (red arrow) versus the other peaks, decreases slightly at the longest reaction time, but it is not clear that the change in the observed relative integrations is

outside of experimental error. At the short times corresponding to those in which the regioselectivity was measured, the isomerization would be negligible.

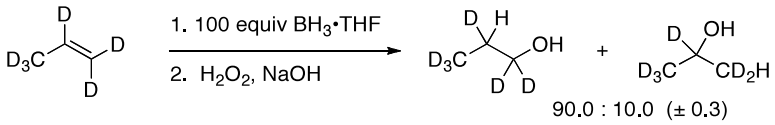


Hours	Sample 1		Sample 2	
	1.5 h	15 h	21 h	47 h
Integrations	6.2	6.2	5.9	5.8
	1	1	1	1
	2.2	2.2	2.1	1.9
	4.2	4.5	4.1	4.0

Figure 2.1. Data for experiment performed to determine isotopic equilibration in the hydroboration of propene-d_6 with BH_3•THF.

The hydroboration of propene-d_6 at 21 °C with 100 equiv of BH_3•THF affords 90.0:10.0 (± 0.3) ratio of primary to secondary alcohols after oxidation. This represents an upper-bound on the selectivity for the BH_3-mediated reaction, since we cannot exclude the contribution of some hydroboration by the more selective alkylboranes. Assuming the applicability of transition state theory, the $\Delta\Delta G^{\ddagger}$ for the transition states leading to the two products would be 1.1 – 1.3 kcal/mol.

Scheme 2.3



A variety of gas-phase computational approaches were explored in an attempt to predict this $\Delta\Delta G^{\ddagger}$. To survey the applicability of methods / basis sets for a broad set of combinations, a series of seven geometries were obtained in a critical area of the energy surface based on an MP2/6-31+G** grid search of the surface. Single point energies were then obtained for each of these structures, along with the MP2/6-31+G** structures of the starting propene and BH_3, in CCSD(T)/aug-cc-pvtz calculations. These energies were then used as the standard for evaluation of simpler combinations of methods and basis sets. Methods / basis sets evaluated in this way include MP2/6-31+G**. MP2/cc-pVDZ, MP2/aug-cc-pvdz, MP2/cc-pvtz, MP2/aug-cc-pvtz, MP4(sdq)/6-31+G**, MP4(sdq)/6-311+G**, MP4(sdq)/cc-pvdz, MP4(sdq)/aug-cc-pvdz, MP4(sdq)/cc-pvtz, MP4(sdq)/aug-cc-pvtz, MP4(sdtq)/6-31+G**, MP4(sdtq)/6-311+G**, MP4(sdtq)/cc-pvdz, MP4(sdtq)/aug-cc-pvdz, CCSD/6-31+G**, CCSD/6-311+G**, CCSD/cc-pvdz, CCSD/aug-cc-pvdz, CCSD/cc-pvtz, CCSD(T)/6-31+G**, CCSD(T)/6-311+G**, CCSD(T)/cc-pvdz, CCSD(T)/aug-cc-pvdz, CCSD(T)/cc-pvtz, B3LYP/6-31+G**, B3LYP/6-311+G**, B3LYP/cc-pvdz, B3LYP/aug-cc-pvdz, B3LYP/cc-pvtz, B3LYP/aug-cc-pvtz, B3LYP/6-31G*, B3LYP/6-31G**, B3LYP/g-31+G*, mPW1K/6-31+G**, B1B95/6-31+G**, TPSS/cc-pvtz, B1LYP/6-311+G**, BLYP/6-311+G**, BP86/6-311+G**, B3PW91/6-311+G**, B3P86/6-311+G**, BHandHLYP/6-311+G**,

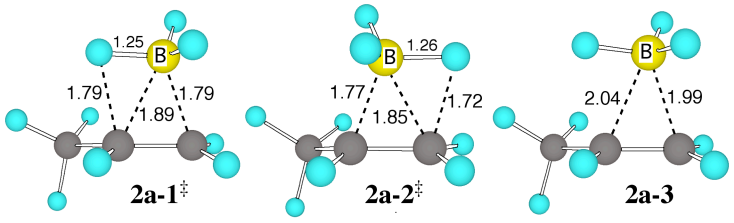
O3LYP/6-311+G**, MPW3LYP/6-31+G**, MPW3LYP/cc-pvtz, and BB1K/6-311+G**, along with a series of 14 home-made functionals involving minor modifications to the B3LYP and mPW1K functionals.

Relative to the CCSD(T)/aug-cc-pvtz standard energies, MP2, mPW1K, B1B95, and TPSS calculations tended to overestimate the energy of the BH_3/propene interaction and overestimated the gradient of the energy in the critical area of the surface. The same was true for calculations employing minor variations from the mPW1K functional. MP4(sdq), CCSD, BLYP, and B1LYP calculations tended to do the opposite, underestimating the energy of the BH_3/propene interaction and underestimating the gradient of the energy as the BH_3 approaches the propene. The MP4(sdtq), B3LYP, and MPW3LYP calculations, as well as CCSD(T) calculations with smaller basis sets, tended to follow closely the CCSD(T)/aug-cc-pvtz standard energies. As examples, in the critical area of the surface, the RMS errors versus the CCSD(T)/aug-cc-pvtz energies were 0.83 kcal/mol for MP2/aug-cc-pvtz, 0.35 kcal/mol for MP4(sdq)/aug-cc-pvtz, 0.08 kcal/mol for MP4(sdtq)/cc-pvdz, 0.19 kcal/mol for B3LYP/6-31G*, 0.45 kcal/mol for CCSD/cc-pvtz, 2.26 for mPW1K/6-31+G**, 2.58 kcal/mol for B1B95/6-31+G**, 0.83 for TPSS/cc-pvtz, and 0.35 kcal/mol for MPW3LYP/6-31+G** calculations. B3LYP/6-31G* was chosen for trajectory calculations and for qualitative and first-approximation explorations of the energy surface because it showed the lowest RMS error among all of the DFT methods / basis sets examined.

Explorations of the potential energy surface in B3LYP/6-31G* calculations identified three key stationary-point structures – transition structure **2a-1**‡ for formation

of the anti-Markovnikov product, transition structure **2a-2**‡ for formation of the Markovnikov product, and the π-complex **2a-3**, arising from complexation of BH_3 to propene, which is the immediate precursor to **2a-1**‡ and **2a-2**‡. CCSD(T)/aug-cc-pvdz calculations were then used to refine the geometries of **2a-1**‡, **2a-2**‡, and **2a-3.** Higher-level single-point calculations were then applied to these refined structures.

The relative energetics of the anti-Markovnikov transition structure **2a-1**‡ and the Markovnikov structure **2a-2**‡ in the high-level single-point calculations, as well as analogous structures optimized in other ways, are summarized in Table **2.2**. All of the calculations, including particularly a converged series of CCSD(T) single –point energies employing very large basis sets, predict an energetic preference for **2a-1**‡ that greatly exceeds that implied by the experimental selectivity. In other words, the experimental reaction is considerably less selective than the 98:2-99:1 expected from the calculations.



We considered many possible reasons for this discrepancy. The simplest possibility, unadorned error in the calculated relative energies, seems doubtful based on the similarity of the structures being compared, the convergence of the results from

various calculational methods, and the quality of the methods employed. A second possibility is that entropy strongly favors **2a-2**‡ in a way that is missed by the often-erring harmonic entropy estimate. The most likely source of an entropy error in the calculations would be the vibrational mode associated with methyl-group rotation. Ordinary calculations treat this mode as a harmonic vibration, but it would more accurately be considered as a hindered rotor. If the barrier for methyl group rotation in **2a-1**‡ versus **2a-2**‡ differed greatly, this could lead to a large error in the calculated entropy.

To address this issue, the second order saddle points corresponding to **2a-1**‡ and **2a-2**‡ with rotation of the methyl group were located in B3LYP/6-31G* calculations along with the corresponding first-order saddle points for BH_3 addition, and the energies of these structures was evaluated in CCSD(T)/cc-pvtz single-point calculations. From these energies, the "barrier" to methyl group rotation was 2.0 kcal/mol in **2a-1**‡ and 1.3 kcal/mol in **2a-2**‡. The free-energy corrections for treatment of these rotations as hindered rotors were taken from the tables provided by Pitzer and Gwinn.[65]This analysis favors **2a-2**‡, but by only 0.1 kcal/mol.

A third possibility is that tunneling favors the Markovnikov process since its barrier is higher. Experimentally, however, there was no apparent difference in the regioselectivity of the reaction of BH_3 versus BD_3 with 1-octene. A one-dimensional infinite-parabola tunneling estimate[66] based on the curvature of the transition vector does favor **2a-2**‡, but by only a rate-factor of 1.28.

Table 2.2. Calculated $\Delta\Delta E^{\ddagger}$ or $\Delta\Delta G^{\ddagger}$ for Transition Structures **2a-1**‡ versus **2a-2**‡ for the Hydroboration of Propene with BH_3.

Method / Basis Set	$\Delta\Delta E^{\ddagger a}$ or $\Delta\Delta G^{\ddagger b}$ (kcal/mol)
B3LYP/6-31G*	2.4[b]
G3B3	2.4[b]
CBS-QB3	2.3[b]
CCSD(T)/cc-pvtz[c]	2.4[a]
CCSD(T)/aug-cc-pvtz[c]	2.4[a]
CCSD(T)/cc-pvqz[c]	2.4[a]
CCSD(T)/aug-cc-pvqz[c]	2.4[a]
BD(TQ)/aug-cc-pvdz[c]	2.6[a]
CCSD(T)/ extrapolated to infinite basis + enthalpy correction – $T\Delta S$	2.5[b,d]
Experiment (assuming transition state theory)	1.1-1.3

[a]$\Delta\Delta E^{\ddagger}$ (as potential energy). [b]$\Delta\Delta G^{\ddagger}$ at 25 °C including harmonic enthalpy and entropy estimates based on the unscaled frequencies. [c]Single point calculations on the CCSD(T)/aug-cc-pvdz structures. [d]MP4/cc-pvdz frequencies were used in the enthalpy and entropy estimates.

A more complex possibility to consider is the role of solvent. We first considered the effect of solvent polarity. Experimentally, solvent polarity has no discernable effect on the regioselectivity.[67] Theoretically, the SCF dipole moments (aug-cc-pvqz) for **2a-1**‡ and **2a-2**‡ are only 3.34 and 2.95 D, respectively, and because the

dipole moment of **2a-1**‡ is greater, solvent polarity should favor **2a-1**‡, not **2a-2**‡. In accord with this, solvent-model calculations (PCM, CPCM, SCIPCM) increase the preference for **2a-1**‡ by 0.3-0.4 kcal/mol, further from experiment.

A second possible role for solvent is the mechanistic complication of a direct transfer of the BH_3 from the solvent as ligand. Brown clearly concluded that free BH_3 is involved in the hydroboration of alkenes,[68] and Brown's observation of a decreased rate in the presence of excess coordinating amine very strongly supports this proposal. However, some observations in the literature have been interpreted as strongly favoring a direct transfer from solvent or ligand as in transition structure **2a-4**‡. In particular, Narayana and Periasamy observed that a small amount of asymmetric induction is observed when prochiral alkenes are hydroborated with BH_3 complexes of chiral amines.[69] Unfortunately, a flaw in such experiments as reported is that the observed products would arise in part from hydroboration by an initially formed chiral mono-alkylborane. Since the dissociation rate or dissociation constant for complexes of chiral mono-alkylborane with chiral amines would differ for the two diastereomeric complexes involved, the observed asymmetric induction could result from the preferential involvement of one of the enantiomeric alkylboranes without any direct involvement of the chiral amine. In this regard, it is notable that the highest asymmetric induction observed by Narayana and Periasamy occurred with unhindered disubstituted reactants that would be expected to involve the greatest amount of hydroboration by initial mono-alkylborane.

Pasto's observation of a negative entropy of activation in kinetic studies also appears to favor a direct transfer from solvent as in transition structure **2a-4**‡. The reported entropy of activation was -27 ± 1 kcal/mol, though a reanalysis of the data reported gives -30.6 ± 2.8. Significant scatter was observed at the replicated central temperature of 25 °C in the study but no replication was carried out for the runs at the temperature extremes of 10 °C and 40 °C. We uncovered a potentially serious problem in failed attempts to carry out kinetics by alternative means – the reaction is exothermic and at the concentrations employed by Pasto the exothermicity raises the temperature by 12°. Most of this heat is generated within 1 second and with the apparatus employed it is questionable that the heat would be dissipated quickly enough for accurate kinetics.

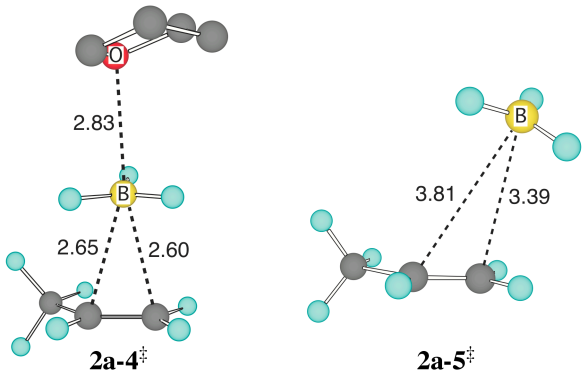
The solvent polarity has no discernable effect on the regioselectivity.[67] However, there is some variation in the reported regioselectivities in the hydroboration of terminal alkenes depending on the detailed solvent/ligand present and reaction conditions, usually within the range 93:7 to 96:4. The interpretation of small regioselectivity differences, observed under synthetically oriented conditions in the literature, is complicated by the potential for varying contributions from reactions of alkylboranes or dialkylboranes. As a result, the variation in the regioselectivity versus solvent is not good evidence for the involvement of solvent-coordinated transition states in the regioselectivity.

Overall, the weight of evidence appears to favor a reaction of free BH_3 under ordinary reaction conditions. While some uncertainty associated with this issue does not affect the key conclusion of the work here, it is of interest to consider in greater detail whether hydroboration occurs via 'free' BH_3 in solution and a transition state resembling

what we will be describing as **2a-5**‡ versus occurring via transfer of the BH_3 from the solvent as ligand. To consider this possibility we wanted to locate a transition structures for BH_3 transfer from THF to propene.

To locate a variational transition state for BH_3 transfer from THF to propene, a series of structures were optimized with a fixed distance between the oxygen of the THF and C1 of propene. Entropy estimates based on the harmonic frequencies were then used to determine the structure with the lowest free energy. The resulting structure **2a-4**‡ is enthalpically 0.4 kcal/mol above a slightly tighter actual saddle point but has a considerable entropic advantage due to lower-energy bending vibrations.

It is important to note that the product from **2a-4**‡ is complex **2a-3**, uncoordinated by THF. In such circumstances the **2a-1**‡ / **2a-2**‡ energy difference would still control the regioselectivity. Notably, the free-energy barrier associated with **2a-4**‡ is predicted to be 2.3 kcal/mol above a dissociative pathway followed by entropic association barrier located, variational transition structure **2a-5**‡ (CCSD(T)/6-31+G**//B3LYP/6-31G*, after allowing for neat THF as its standard state).



2a-4‡ **2a-5**‡

The starting point for the location of **2a-5**‡ was the lowest-energy structure found in a scan of positions with BH_3 and propene centroids separated by 5 Å. From this structure, a steepest-descent path in mass-weighted coordinates was followed. The steepest-descent path was obtained using a modified version of the program PROGDYN in which no momentum is given to nuclei and very small steps (< 0.00025 Å) are used, varying the size of the steps continually to avoid oscillations. This approach has the problem of being extremely slow compared to other approaches, but it has the virtue of being extremely reliable. The path obtained consisted of 7908 points. At regular intervals along the steepest-descent path, frequency calculations were carried out and free energies were calculated using the harmonic approximation without scaling. Structure **2a-5**‡ was the free energy maximum along this path.

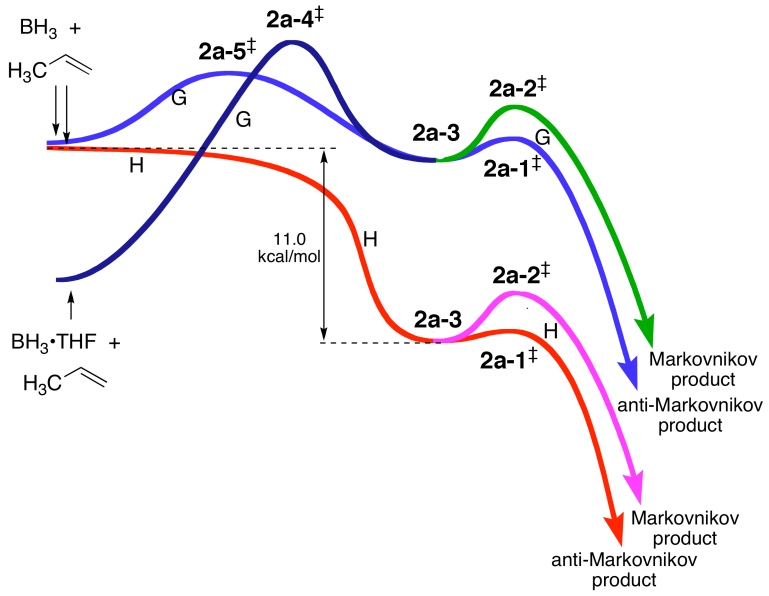


Figure 2.2. Reaction coordinate diagram. Harmonic Gibbs free energy (G) and harmonic enthalpy (H) were estimated at 25 °C.

Consideration of the reaction energetics suggests an explanation for the inability of transition state theory to account for the product ratio. Figure **2.2** shows the enthalpic and free-energy profile in two dimensions, while Figure **2.3** shows a three-dimension picture of the potential energy surface. Calculationally, the formation of **2a-3** from BH_3/propene is enthalpically barrierless (Figure **2.3**). This fits with the experimentally observed barrier of 2 ± 3 kcal/mol for the hydroboration of ethylene in the gas phase.[40] Calculationally, the complexation is downhill by 11.0 kcal/mol in CCSD(T)/aug-cc-pvqz calculations including a harmonic enthalpy estimate. Considerable excess energy is thus available from the formation of **2a-3**, and the barriers for formation of products from **2a-3** are quite small – **2a-1**‡ is only 0.8 kcal/mol above **2a-3** in free energy. Under these circumstances, we considered that trajectories may pass to product faster than thermal equilibration with solvent.

To explore this idea, a series of classical trajectory studies were performed (Table **2.3**), including B3LYP/6-31G* trajectories started directly from **2a-3**, **2a-4**‡, and **2a-5**‡, and ONIOM (B3LYP/6-31G*:AM1) trajectories started from **2a-4**‡ or **2a-5**‡ in a bath of 18 THF molecules confined to a 14 Å cubic box after a 500 - 8500 fs equilibrations. Trajectories started from **2a-3** statistically at 25 °C, i.e., with no excess energy, underwent addition with a half-life of ≈700 fs and afforded ≈1% of the Markovnikov product. Figure **2.4** shows the decay of complex to products over time; the decay follows first-order exponential with $k = 9.8 \times 10^{11}$. The selectivity observed in the trajectories started from the complex fits quite well with transition state theory, though not with experiment. This observation notably weighs against recrossing or

unknown subtle classical entropy effects as the source of the discrepancy between experiment and the selectivity predicted from transition state theory. In contrast, the trajectories started from points before **2a-3** on the reaction coordinate, thus having excess energy in the area of **2a-3**, afforded 10-12% of the Markovnikov product. This fits strikingly well with experiment.

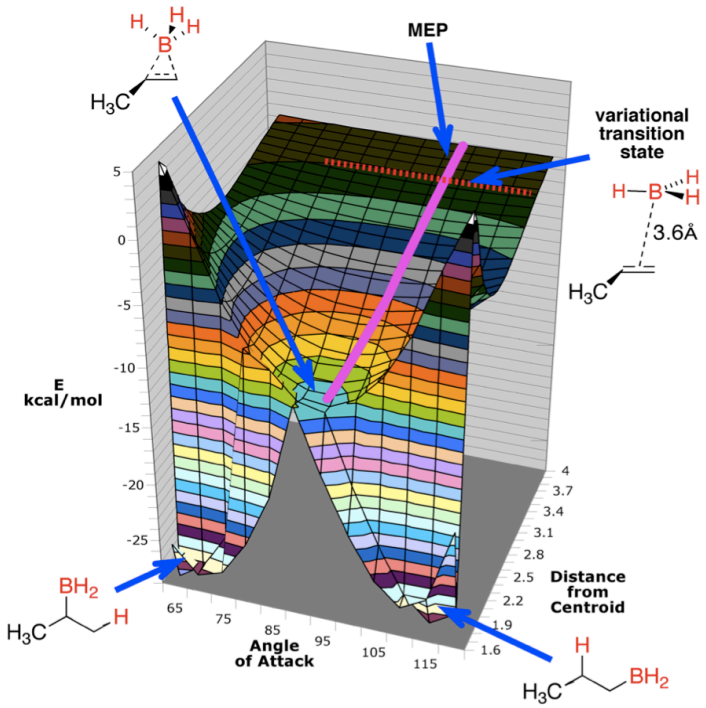


Figure 2.3. 3-dimensional B3LYP/6-31G* potential energy surface. The energy was obtained for different angles and distances from a crude centroid 0.7 Å from middle carbon. This represents the enthalpically barrierless approach of the BH_3 to the propene in many ways ending in the formation of a bowl like area around π-complex **2a-3**. To exit the area it could be by passing though the shallow part of the bowl following the minimum energy path (MEP). Though this path the barriers for formation of products from **2a-3** are quite small compared to the formation of product from either very small or very large angles of attack.

The trajectories employed above are classical, i.e., without zero-point energy. For trajectories starting from **2a-3**, **2a-4**‡, or **2a-5**‡, the desired energy in each of the normal modes was mapped from a random number generator to a Boltzmann distribution. The phase of each of the normal modes was mapped from Gaussian distribution of random numbers. This distribution is not correct for a classical oscillator but would be approximately correct for a quantum oscillator in its ground state (only ignoring mode displacements outside of the classical limit), and has the advantage that a larger portion of the trajectories start with an energy approximating the initially desired energy. After an energy / force calculation on the initial geometry, the total initial energy was calculated and the trajectory was thrown out if the energy did not agree satisfactorily with the desired energy. (This is a variation of the conventional practice of scaling energies).

For the ONIOM trajectories in THF, initial structures were generated by a series of cycles of simulated annealing followed by minimization, choosing the lowest-energy structure obtained as the starting point for further trajectories (Table **2.3)**. It should be noted that this structure is very unlikely to be a global minimum, and the subsequent trajectories will in principle be too high in energy by the amount to which the starting structure in not optimum. In practice, this probably does not matter because the error is divided up among the many degrees of freedom and is small compared to the normal thermal energy present. Trajectories for **2a-5**‡ + 18 THF molecules or **2a-4**‡ + 17 THF molecules were then initiated as above, only with no displacement of the phases of the normal modes and initially fixing the B-C1 and B-C2 distances. For the **2a-5**‡ / 18 THF

trajectories, the B-C1 and B-C2 distances were released after 500 fs. For the **2a-4**‡ / 17 THF trajectories, the trajectories were continued for 8500 fs and sampled every 500 fs starting at 1000 fs. For the sampled points, the B-C1 and B-C2 distances were released and the trajectories were followed until product formation or a 5000-fs time limit.

Table 2.3. Classical Trajectory Studies.

Starting point	Anti-Markovnikov	Markovnikov	Unreactive in 5000 fs
2a-3	513	5	2
2a-4‡	338	47	496[a]
2a-5‡	739	110	465
2a-5‡ + 18 THF, equilibrated[b]	76	9	17[a]
2a-4‡ + 17 THF, equilibrated[c]	19	2	3[a]

[a]Includes trajectories affording THF•BH_3. [b]500 fs equilibrations before releasing a fixed B-C distance. [c]1000 -8500 fs equilibrations before releasing a fixed B-C distance.

A more detailed understanding of the regioselectivity can be gleaned from considering the time-course of the selectivity for trajectories started from **2a-5**‡. For the 25% of trajectories that afford product within 800 fs, the amount of Markovnikov product is particularly high (21%). The selectivity is higher for the 39% of trajectories that afford product in the 800 – 5000 fs range, with 7.5% Markovnikov addition. Figure 2.4 shows the selectivity of the reacted trajectories over time, illustrating how fewer

products are formed over time and how the selectivity increases as the excess energy equilibrates within the molecule. An RRKM calculation based on the energy difference between **2a-5**‡ and **2a-3** predicts 7.4% of the Markovnikov product. RRKM theory predicts the rate of chemical reactions at a given energy.[70] The described RRKM calculation was carried out using an available program[71] and employing the Beyer-Swinehart direct-count algorithm.[72] The complex **2a-3** was used as the starting material for the rate calculations and the energy employed was 6.6 kcal/mol, the energy difference between **2a-5**‡ and **2a-3** at B3LYP/6-31G*, as is reasonably appropriate for comparison with B3LYP/6-31G* trajectories. It may be noted that the actual excess energy when **2a-3** is formed in solution is not easily defined.

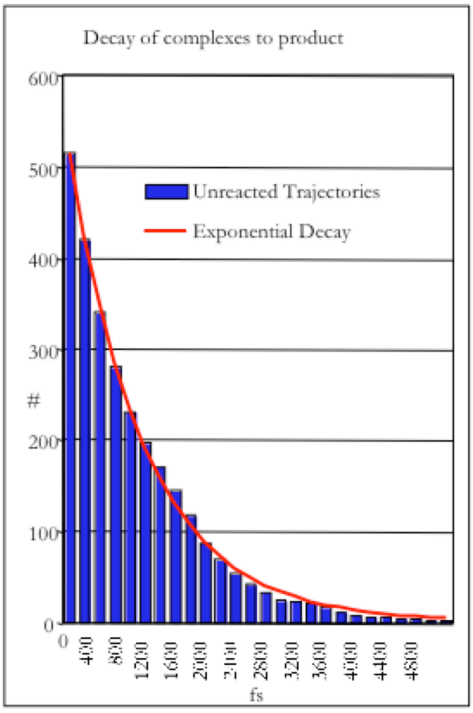


Figure 2.4. The selectivity of the reacted trajectories over time.

From the observations in the trajectories and the RRKM theory predictions, we envision the selectivity in solution as involving three stages: a 'direct-trajectory' stage, with low selectivity, an RRKM stage, with medium selectivity, and a thermally-equilibrated stage, developing over several picoseconds as the excess energy is transferred to solvent. This last stage should be quite selective, as evidenced by the results with trajectories starting from **2a-3**, but by then the damage is done.

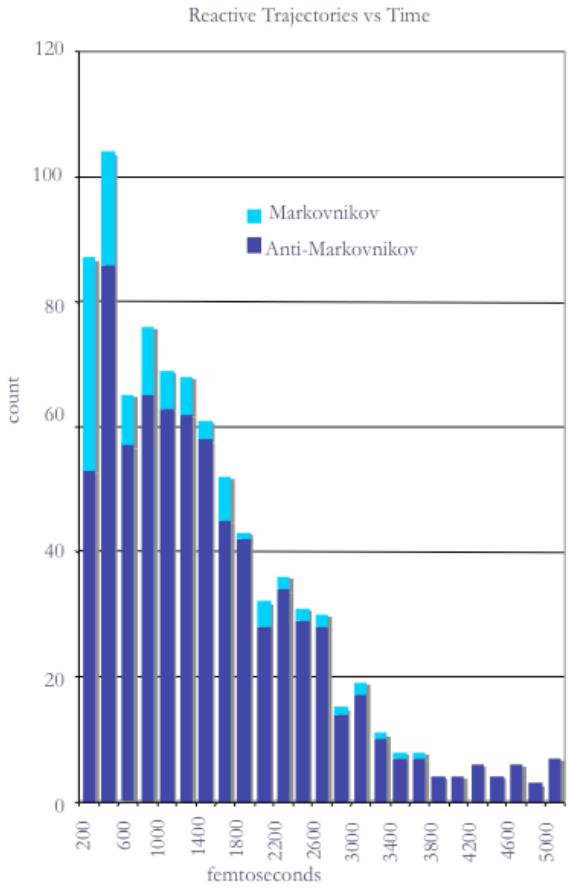
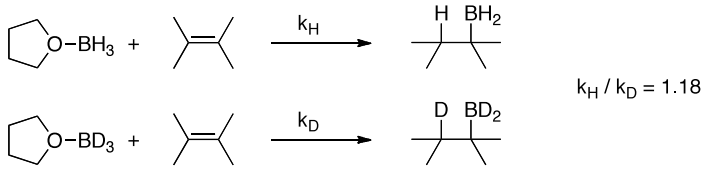


Figure 2.5. The selectivity of the reacted trajectories over time.

Some unusual experimental observations in hydroboration support the mechanistic picture here. In particular, hydroboration has long been recognized as "remarkably insensitive to major changes in the structure of the olefin", a factor in its broad utility, and it exhibits an equally remarkably low intermolecular H/D isotope effect of 1.18 (Scheme **2.4**). This unusual isotope effect observed in the literature as well as a new isotope effect obtained in the current study requires comment.

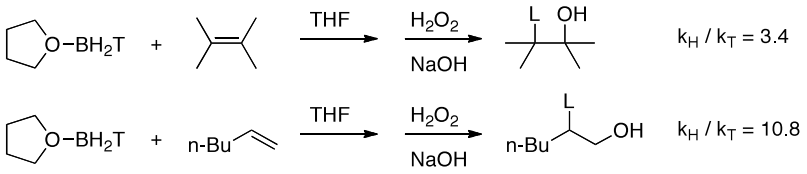
Pasto had reported isotope effects for hydroboration determined in two ways.[39] The first was determined by absolute kinetics for the reaction of BH_3 or BD_3 with 2,3-dimethyl-2-butene. This result should reflect the rate-limiting step for the hydroboration, and the quite small isotope effect observed, 1.18, fits well qualitatively with a rate-limiting transition state resembling **2a-5**‡ as proposed here.

Scheme 2.4



The second way is which Pasto measured the isotope effect was based on product analysis after hydroboration with partially tritiated borane. The isotope effect obtained in this way involves an *intramolecular* competition between H and T, and reflects the isotope effect for the product-determining step (Scheme **2.5**).

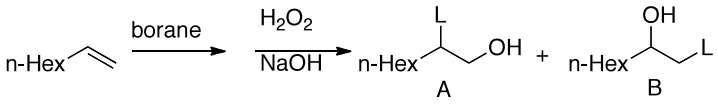
Scheme 2.5

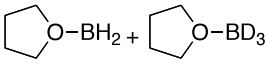
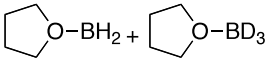
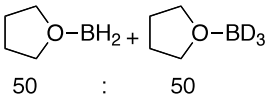
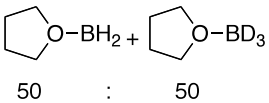


The significance of the greatly differing isotope effects obtained by absolute kinetics versus intramolecular competition would not have been obvious at the time of these studies. As became apparent from later mechanistic studies in other systems,[73] such a discrepancy is indicative of separate rate-limiting and product-determining steps in a mechanism. Pasto's isotope effects thus supported the mechanistic proposal of Klein discussed in the introduction, but he was not able to recognize this at the time.

This issue is complicated by an intramolecular competition isotope effect determined for the current study. In this measurement, partially deuterated 1-octanol was produced by the hydroboration of 1-octene with partially deuterated 1-octene. The deuterium content of the 1-octanol produced when the borane was in excess was compared with the deuterium content obtained when the 1-octene was in excess. (In this latter case, all of the active H and D (~9:1) in the borane end up in the product, so the product acts as a measure of the content of the original borane.) From this measurement, an isotope effect of 1.15 ± 0.10 was obtained. Because k_H/k_T should exceed k_H/k_D by only a limited extent,[74, 75] the Pasto isotope effect and the isotope effect here are inconsistent. The origin of this discrepancy is unknown, but the isotope effect determined here is qualitatively consistent with a low selectivity decided in a dynamically controlled process.

Table 2.4. Intramolecular competition isotope effect determined for the current study.

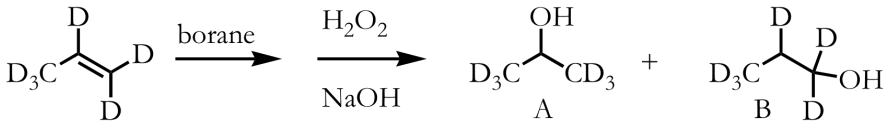


borane	equivalents of octene	% of A	% of B	k_H / k_T
 9 : 1	3	6.4	93.6	1.5
 9 : 1	0.3	6.2	93.8	
 50 : 50	3	11.1	88.9	0.66
 50 : 50	0.3	7.0	93.0	

The Isotope effect was also measured with a 1 : 1 ratio of H to D. An isotope effect of 0.66 was obtained. This is not consistent either with a normal primary H/D isotope effect. For the 1 : 1 ratio of H to D in a sample of borane, it was assumed that the isotopes were statistically distributed at equilibrium. With the assumption, the ratio of BH_3 : BH_2D : BHD_2 : BD_3 would be 1 : 3 : 3 : 1. In a non-Curtin-Hammett situation in which a rate-limiting step committing a molecule of borane to reaction (calculationally, formation of a borane-alkene complex) precedes a product-determining step that decides whether H or D ends up in the product alcohol, 12.5% of the reaction would result from BH_3, 37.5% of the reaction would result from BH_2D, 37.5% of the reaction would result

from BHD_2, and 12.5% of the reaction would result from BD_3. For an intramolecular isotope effect k_H/k_D, the relative amount of product from reaction of an H would be 0.125 (from BH_3) + 0.375 x (2 / (2 + 1/(k_H/k_D))) (from BH_2D) + 0.375 x (1 / (1 + 2/(k_H/k_D))) (from BHD_2). The relative amount of product from reaction of a D would be 0.125 (from BD_3) + 0.375 x ((1/(k_H/k_D)) / (2 + 1/(k_H/k_D))) (from BH_2D) + 0.375 x (2/(k_H/k_D) / (1 + 2/(k_H/k_D))) (from BHD_2). As an example, if the intramolecular isotope effect k_H/k_D were 3, the H product would be 0.125 + 0.3214 + 0.225 and the D product would be 0.125 + 0.0536 + 0.15, and the H/D ratio would be 2.04.

Table 2.5. Regioselectivity of the hydroboration of propene-d_6 with BH_3 at different temperatures.



Borane	Solvent	Temp. °C	equivalents of borane	% of A	% of B
BH_3	THF	25	100	10.0	90.0
BH_3	THF	45	100	10.6	89.4
BH_3	THF	70	100	11.2	88.8

A new unusual observation is that the regioselectivity is surprisingly temperature-insensitive – hydroboration of propene-d_6 at 21, 45 and 70 °C afforded 10.0, 10.6 and 11.2% Markovnikov addition (Table **2.5**), respectively. This corresponds to a

$\Delta\Delta H^{\ddagger}$ of only 0.5 ± 0.2 kcal/mol. These observations were shoehorned into a conventional mechanistic picture, though in retrospect they clearly contradict it.

In conclusion, current understanding of selectivity in ordinary chemical reactions assumes the applicability of the transition state theory model of reactivity. It is found here that transition state theory fails in an example where it is ubiquitously invoked, the hydroboration of alkenes with BH_3. High-level *ab initio* calculations predict too large of an energy difference between competitive transition structures to account for the observed product ratio, and the consideration of calculational error, solvent, tunneling, and entropy effects does not resolve the discrepancy. Trajectory studies, however, predict well the experimental selectivity. This means that in this most 'textbook' of reactions, transition state theory fails and the selectivity can only be understood by consideration of dynamic trajectories.

CHAPTER III

ISOTOPE EFFECTS, DYNAMICS, AND THE NATURE OF SELECTIVITY IN THE HYDROBORATION OF STYRENE

Introduction

Most intermediates in chemical reactions are initially formed with substantial excess energy. This is due to short time scale of reaction coordinates; as a molecular geometry passes from the area of an initial transition state toward the area of an intermediate, potential energy is lost but there is far too little time, typically 50 to 200 fs, for thermal equilibration in solution. As a result, an intermediate is formed with an available energy that is approximately its difference in energy versus the preceding transition state. If this excess energy is lost by thermal equilibration with the medium faster than any subsequent step in the mechanism, then the energy will have no effect. This is the most common case for reactions in solution, and such thermal equilibration is routinely implicitly assumed when the rates and selectivities of subsequent steps are interpreted using transition state theory. A second possibility, common in gas phase reactions, is that the excess energy becomes equilibrated within the molecule (by intramolecular vibrational-energy redistribution, IVR) without being lost to the medium prior to the next step in the mechanism. In such cases, the allowance for the excess energy in RRKM theory allows the understanding of subsequent reactivity and selectivity.

A third possibility presents a more difficult problem for chemistry. The initial

excess energy in an intermediate will not be statistically distributed between the vibrational modes. If subsequent steps occur on a time scale that is faster than or competitive with IVR, then theory provides less guidance on the rates and selectivities of the next steps. The branching ratio among possible reaction pathways may defy both statistical expectations and intuition, for example when an apparently symmetrical intermediate does not proceed equally along apparently equivalent pathways.[49,53-58,60-61,76] The importance of this phenomenon in organic reactions has been particularly highlighted by the work of Carpenter and coworkers. Most importantly, these effects can influence reactions in which the trajectories pass through a flat area on the potential energy surface,[56-58,60-61,76e-h,77] or can by-pass minimum on the reaction coordinate.[77-78]

When trying to understand selectivity, prior to Carpenter's work, it has traditionally been assumed that separate products arise from separate transition states. Though this assumption has been considered to be a rule and it has been shown to be not be reliable for all of the cases mentioned above for the last few decades.[79] For example, in the case of a bifurcating energy surface, reactants that pass through a rate-limiting transition state can proceed to two products to equally yield two equivalent products. There have been many theoretical studies on bifurcating surfaces that involve symmetry breaking.[79g,80] The selectivity in this class of reactions is 1:1 with a mixture of indistinguishable products or enantiomers.

There are also examples of unsymmetrical bifurcating surfaces where the minimum free energy path (MEP) does not bifurcate and trajectories may lead to two distinct products. Transition state theory currently cannot predict the product mixture

and therefore, trajectory calculations are required.

Transition state theory is only capable of predicting the sum of the rate constants for two reactions after branching between product channels after the rate-limiting transition state. However, transition state theory has been proven to work very well in many cases to predict branching after the rate-limiting step, due to the fact that relaxation is faster than subsequent reactions in most instances. In some cases with experimental evidence, transition state theory has been experimentally proven to make incorrect predictions because the relaxation or lost of energy to solvent is slower than the branching toward products. An approach to this problem has recently been suggested by Truhlar, who has been able to predict branching ratios of reactions when a reaction path branches after a point where branching between product channels after the rate-limiting transition state, including cases where intermediates occur. This was proposed in order to estimate the branching fraction of the hydroboration of propene, after it was concluded by us that "transition state theory fails and the selectivity can only be understood by consideration of dynamics trajectories (Chapter II)" and that "reactions exhibiting dynamic effects, chemistry must develop new qualitative ideas to account for reactivity and selectivity".[81] The new method is centered on the combination of non-statistical phase space theory for a direct component with VTS theory for the indirect component. There methods allow one to understand the effects that influence a reaction and allow the use of high-level electronic structure methods for complex reaction systems.

Truhlar was able to propose a qualitative theory that did not involve the use of dynamical trajectories that includes the experimental branching ratio. When a reaction progresses along a reaction pathway it partially equilibrates by IVR. At this point an indirect mechanism can occur where some of the reactants reach equilibrium as an intermediate and is directed by the two transition states that lead to two products. On the other hand, the other portion of the reaction can maintain some excess energy allowing them to pass the second point where branching between product channels after the rate-limiting transition step. Truhlar's model represents a mixture of the indirect mechanism (requires TST) and the direct mechanism (requires non-statistical phase space theory) and the newly developed model is referred to as "canonical competitive non-statistical model (CCNM). This Thuhlar methodology was put forward as a possible way to treat our observations for the hydroboration of terminal alkenes with BH_3 and the calculated results were closely in agreement with the experimental selectivity.

These observations leave some key questions in place. Of particular importance is the breadth of reactions affected by the phenomenon observed in the simple hydroboration. Do experimental observations in the other terminal alkenes hydroborations suggest the same effect? If some do and some do not, what can be learned about when statistical rate theories are applicable and when they are should be expected to fail?

To address these issues, we have explored the role of dynamic effects in the styrene hydroboration reaction by a combination of experimental and calculational studies.

Experimental Selectivity and Computational Research Strategy

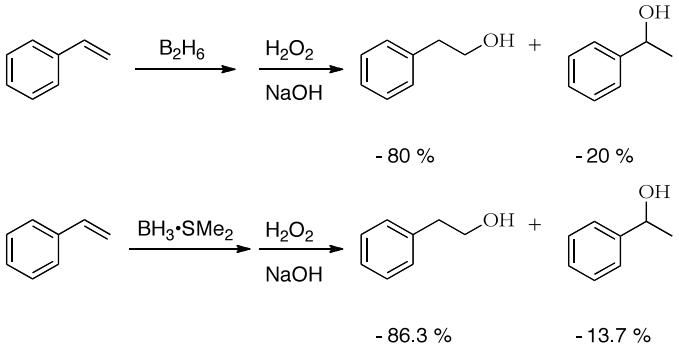
In approaching the question of whether dynamic effects are important in the hydroboration of particular alkenes with BH_3, one must first resolve the actual experimental selectivity in the BH_3 reaction. A substantial complication is that the selectivity as it is normally observed may be a composite of up to three separate steps - hydroboration by BH_3, hydroboration by RBH_2, and hydroboration by R_2BH. When unhindered, the intermediate alkylboranes are more reactive,[16] but they are more regioselective as well, so the initial reaction of BH_3 should be less selective than the composite ratio. In cases the selectivity of the BH_3 step may be discerned or extrapolated from literature data. Where practical, we have measured the selectivity by the approach of using very large excesses of BH_3 with the goal of minimizing the contribution of hydroborations by alkylboranes and dialkylboranes to the overall selectivity. In other cases, the selectivity with BH_3 is only known approximately.

After resolving the experimental selectivity for particular reactions, we will consider whether predictions based on transition state theory accurately account for the selectivity. This requires accurate computational methodology. We had previously examined 61 combinations of *ab initio* or DFT methods and basis sets in their ability to model the potential energy surface for addition of BH_3 to propene, as judged by comparison with CCSD(T)/aug-cc-pvtz energies.[82] We have since examined additional methods, such as M06-2X. B3LYP/6-31G* calculations performed the best among DFT functionals / basis sets tested, and were used here for geometry optimizations and trajectory calculations. For more accurate energies, G3B3 calculations were found to

perform best among higher-level methods that are applicable to the larger systems studied here.[83] CCSD(T) calculations with as large of basis set as practical were also carried out on many structures of interest, and these were uniformly consistent with the G3B3 results. G3B3 energies matched those found in CCSD(T)/aug-cc-pvqz calculations within 0.1 kcal/mol, making it ideal for the study of BH_3/Styrene, which is a larger system.

When transition state theory does not appear to accurately predict the experimental selectivity, we will consider whether a more accurate prediction can be made employing dynamic trajectories.

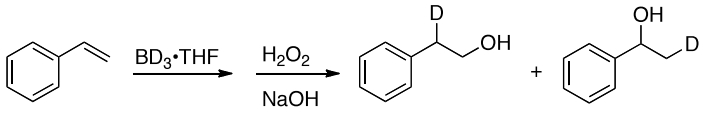
Scheme 3.1



The hydroboration of styrene is relatively unselective with BH_3. Brown and Zweifel reported an 80:20 mixture of anti-Markovnikov and Markovnikov using in situ-generated borane in diglyme at 20 °C,[14] while Lane reported an 86:14 mixture using

borane – methyl sulfide in hexane.[67] Under conditions precluding trialkylborane formation ($LiBH_4$ / ethyl acetate in ether, 25 °C), the selectivity was only 77:23.[68a]

Scheme 3.2



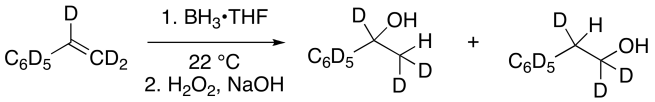
0.3 equiv BD_3 83.8 : 16.2

44 equiv BD_3 80.6 : 19.4

Our strategy of using larges excesses of BH_3•THF to minimize the contribution of hydroboration by alkyl- and dialkylboranes to the observed regioselectivity runs into some problems in practice. One problem is that small amounts of impurities in the BH_3•THF, for example from THF decomposition, can interfere with the analysis. A second concern was that selective loss of the minor regioisomer could occur during the workup and extraction procedure. These concerns showed when the reaction was first attempted using 0.3 and 44 equivalents of BD_3•THF and analyzed by ^1H NMR. However, ^2H NMR analysis allow the estimate of the regioselectivity to be 83.8:16.2 in the case of 0.3 equiv and 80.6:19.4 for an excess of 44 equiv. The reproducibility of the first analyses was not as high as desired, and it proved advantageous to study the reaction of stryrene-d_8. This allows the direct observation of the regioselectivity in the oxidized reaction mixture by ^2H NMR. It also allowed a reconfirmation of the regioselectivity since two peaks from each product were analyzed. At 22 °C, the selectivity was 83:17 when an excess of styrene was used but this decreased to 80:20

when 44 equiv of BH_3•THF versus styrene and 77:23 with 100 equiv of BH_3•THF. The differing product ratios with 44 versus 100 equiv of BH_3•THF suggest that a limiting ratio may still not have been reached. The use of larger excesses was impractical, and the 77:23 ratio is best considered as an upper limit to the selectivity with BH_3. This corresponds to a phenomenological $\Delta\Delta G^{\ddagger}$ of 0.7 kcal/mol.

Scheme 3.3



0.3 equiv BH_3 83 : 17

44 equiv BH_3 80 : 20

100 equiv BH_3 77 : 23

As previously found with propene, there is no enthalpic barrier for formation of the olefin – BH_3 π-complex **3a-2** from separate styrene and BH_3 molecules. A variational transition state (**3a-5**‡) for the association of BH_3 with styrene to afford the π-complex was located by an adaptation of the "nosaddle" procedure of Truhlar and coworkers.[83, 84] The starting point for the location of **3a-5**‡ was the lowest-energy structure found in a scan of positions with BH_3 and styrene separated by 5 Å. From this structure, a steepest-descent path in mass-weighted coordinates was followed using the program PROGDYN and structure **3a-5**‡ was the free-energy maximum along this path. Relative to separate starting materials the entropic association barrier, structure **3a-5**‡, is 5.7 kcal/mol. From π-complex **3a-2**, the two transition structures **3a-3**‡ and **3a-4**‡ lead to

the regioisomeric products. The barriers associated with these structures are very small. Both structures are of course higher in potential energy than **3a-2**. However, due in large part to the neglect of the enthalpy associated with the reaction coordinate, the calculated formal enthalpy of **3a-3**‡ is lower than that of **3a-2**. Both structures would represent dynamical bottlenecks on the way to the products, but the G3B3-predicted free-energy barriers are only 1.1 and 2.3 kcal/mol for **3a-3**‡ and **3a-4**‡, respectively. This energetics are clearly pictured in the reaction coordinate diagram below, Figure **3.1**.

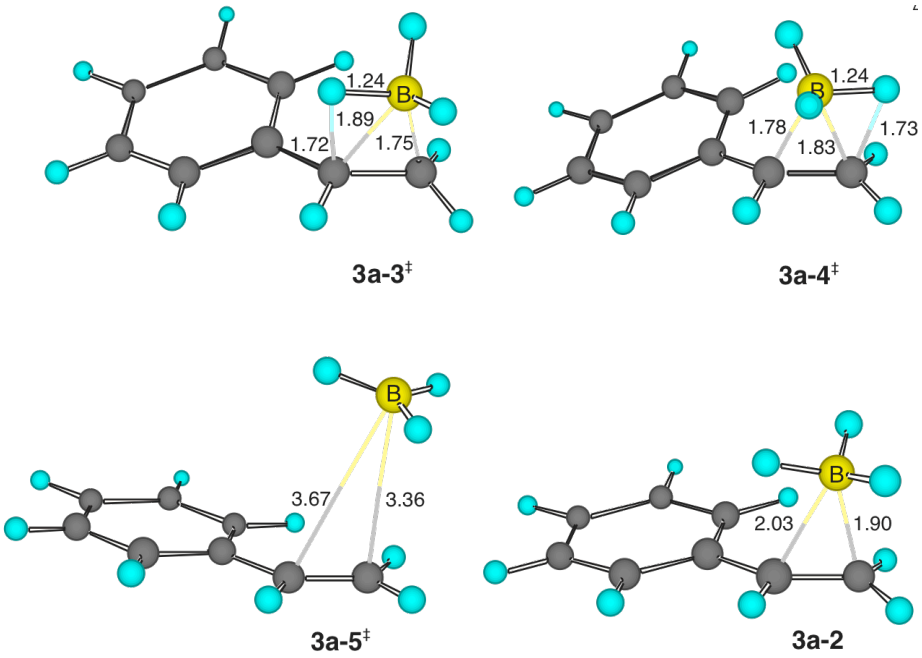


Table 3.1. Enthalpies and free energies of structures located for the hydroboration of Styrene with BH_3

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
3a-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
3a-5‡	$\Delta G^{\ddagger} = 5.7$ $\Delta H^{\ddagger} = -2.7$	$\Delta G^{\ddagger} = 6.4$ $\Delta H^{\ddagger} = -2.2$	$\Delta G^{\ddagger} = 6.2$ $\Delta H^{\ddagger} = -1.5$
3a-2	$\Delta G = 1.1$ $\Delta H = -9.3$	$\Delta G = 3.6$ $\Delta H = -9.4$	$\Delta G = 5.0$ $\Delta H = -7.7$
3a-3‡	$\Delta G^{\ddagger} = 2.3$ $\Delta H^{\ddagger} = -9.6$	$\Delta G^{\ddagger} = 5.2$ $\Delta H^{\ddagger} = -8.6$	$\Delta G^{\ddagger} = 6.2$ $\Delta H^{\ddagger} = -7.2$
3a-4‡	$\Delta G^{\ddagger} = 3.5$ $\Delta H^{\ddagger} = -8.2$	$\Delta G^{\ddagger} = 6.7$ $\Delta H^{\ddagger} = -6.9$	$\Delta G^{\ddagger} = 7.7$ $\Delta H^{\ddagger} = -5.6$
3a-6	$\Delta G = -18.5$ $\Delta H = -28.1$	$\Delta G = -16.2$ $\Delta H = -29.2$	$\Delta G = -14.4$ $\Delta H = -27.1$
3a-7	$\Delta G = -18.5$ $\Delta H = -29.6$	$\Delta G = -15.2$ $\Delta H = -30.0$	$\Delta G = -13.6$ $\Delta H = -28.1$

The enthalpies and free energies were estimated using method/basis set G3B3, B3LYP/6-31G*, B3LYP/6-31+G**, they are relative to separate starting materials and express in kcal/mol.

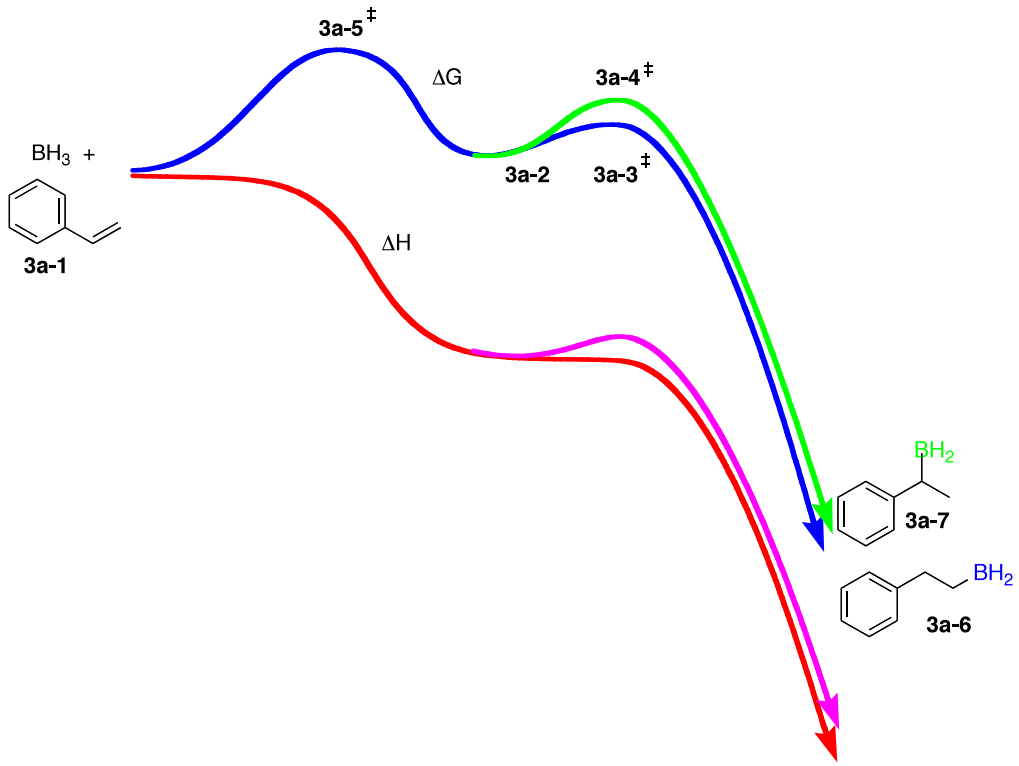


Figure 3.1. G3B3 ΔH and ΔG reaction coordinate diagrams for structures located for the hydroboration of Styrene with BH_3.

Because the consideration of whether transition state theory is making accurate predictions often hinges on relatively small energy differences, second-order perturbative anharmonic contributions to the vibrational energies and entropy were calculated[85] for each structure and applied as corrections to all enthalpies and free energy (Table **3.2**). The barriers associated with these structures are still very small. Even after correction we observe that both structures would represent dynamical bottlenecks on the way to the products. The corrected G3B3-predicted free-energy barriers are only 1.8 and 3.6 kcal/mol for **3a-3**‡ and **3a-4**‡, respectively. Strikingly, there is no enthalpic barrier for formation of transition state **3a-3** from π-complex **3a-2,** even

after the correction this is downhill by 0.3 kcal/mol. For the formation of transition state **3a-4**‡, the corrected enthalpic barrier is only 1.1 kcal/mol.

Table 3.2. Enthalpies and free energies of structures located for the hydroboration of Styrene with BH_3 after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
3a-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
3a-2	$\Delta G = 0.3$ $\Delta H = -9.4$	$\Delta G = 2.7$ $\Delta H = -9.5$	$\Delta G = 4.1$ $\Delta H = 7.8$
3a-3‡	$\Delta G^{\ddagger} = 1.8$ $\Delta H^{\ddagger} = -9.7$	$\Delta G^{\ddagger} = 4.7$ $\Delta H^{\ddagger} = -8.7$	$\Delta G^{\ddagger} = 5.7$ $\Delta H^{\ddagger} = -7.3$
3a-4‡	$\Delta G^{\ddagger} = 3.6$ $\Delta H^{\ddagger} = -8.3$	$\Delta G^{\ddagger} = 6.8$ $\Delta H^{\ddagger} = -6.9$	$\Delta G^{\ddagger} = 7.8$ $\Delta H^{\ddagger} = -5.6$
3a-6	$\Delta G = -19.4$ $\Delta H = -28.8$	$\Delta G = -17.1$ $\Delta H = -30.0$	$\Delta G = -15.3$ $\Delta H = -27.8$
3a-7	$\Delta G = -19.4$ $\Delta H = -29.6$	$\Delta G = -15.9$ $\Delta H = -30.1$	$\Delta G = -14.3$ $\Delta H = -28.2$

The enthalpies and free energies were estimated using method/basis set G3B3, B3LYP/6-31G*, B3LYP/6-31+G**, they are relative to corrected separate starting materials and express in kcal/mol.

The difference between the predicted $\Delta\Delta G^{\ddagger}$ of 1.8 kcal/mol and the experimental value of 0.7 kcal/mol is small, and it must be considered in detail what level of evidence this provides, *if any*, for the inaccuracy, or more precisely, *inapplicability* of transition state theory to the understanding of the product ratio. In the hydroboration of propene, the G3B3 energy differences between Markovnikov and anti-Markovnikov transition structures were found to match quite closely with other high-level calculations, including CCSD(T) calculations employing very large basis sets. However, a simple error of 1.1 kcal/mol in the relative energies of the transition structures cannot be directly excluded.

Due to the negligible barrier associated with transition structure **3a-3**‡ versus complex **3a-2** (0.4 kcal/mol on the vibrational ground-state surface), tunneling should contribute little to the rate of the anti-Markovnikov process. However, the larger barrier associated with transition structure **3a-4**‡ could be more accelerated by tunneling. A one-dimensional truncated parabola estimate of the tunneling based on the curvature of the transition vectors (448*i* and 503*i* for **3a-3**‡ and **3a-4**‡, respectively) favors **3a-4**‡ by a factor of 1.21. Allowance for this factor has the effect of decreasing the difference between theory and experiment by 0.1 kcal/mol.

Taking into account each of these factors in the predicted $\Delta\Delta G^{\ddagger}$ for **3a-3**‡ and **3a-4**‡ suggests no explanation for the inability of transition state theory to account for the product ratio. To find an explanation for the product ratio it was necessary to pay close attention to the reaction energetics. Figure **3.2** shows the enthalpic and free-energy profile for the hydroboration of styrene with BH_3 in two dimensions, while Figure **3.3** shows a three-dimension picture of the potential energy surface. Calculationally, the

barrier for the association of styrene and BH_3, variational transition structure **3a-5**‡, is 5.7 kcal/mol. As a result, considerable excess energy is thus available from the formation of **3a-2**, and the barriers for formation of products from **3a-2** are quite small – **3a-3**‡ has no enthalpic barrier. Under these circumstances, we considered that trajectories might pass to product faster than thermal equilibration with solvent.

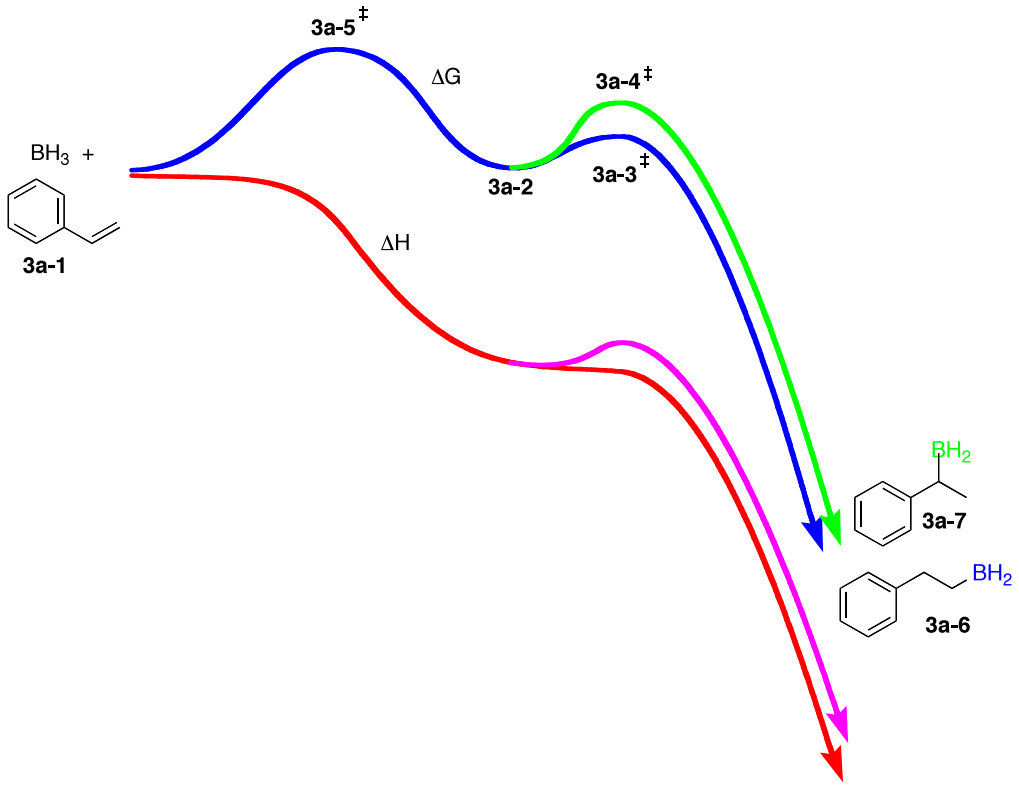


Figure 3.2. G3B3 ΔH and ΔG reaction coordinate diagrams for structures located for the hydroboration of Styrene with BH_3 after anharmonic corrections.

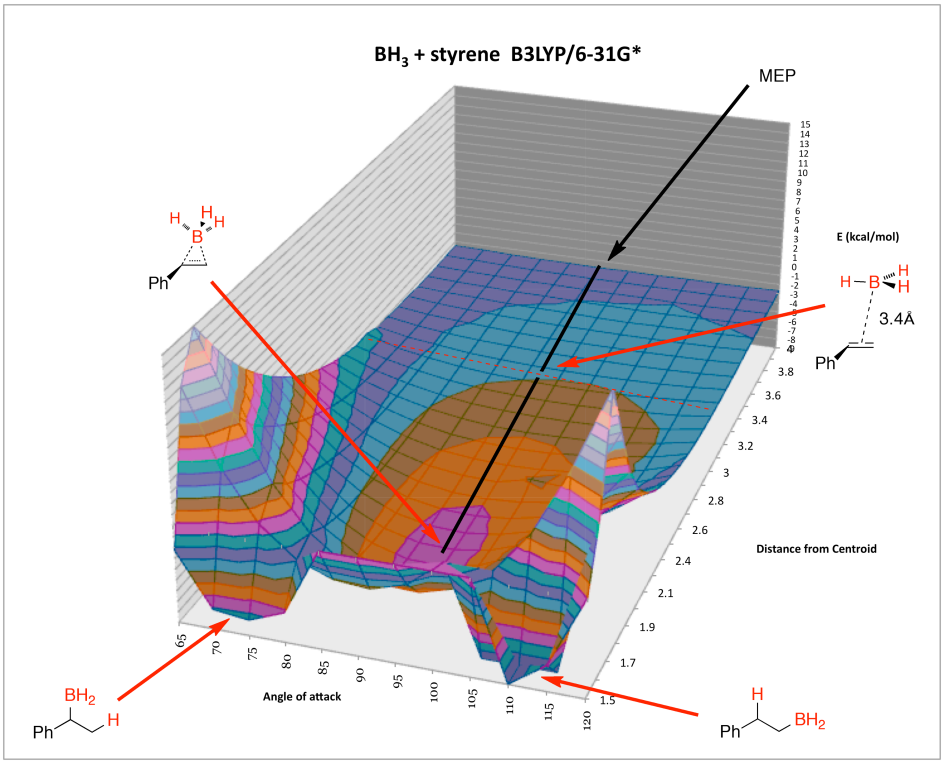


Figure 3.3. 3-dimensional B3LYP/6-31G* potential energy surface. [a]The energy was obtained for different angles and distances from a crude centroid from middle carbon. This represents the enthalpically barrierless approach of the BH_3 to the propene in many ways ending in the formation of a bowl like area around π-complex **3a-2**. To exit the area it could be by passing though the shallow part of the bowl following the minimum energy path (MEP). Though this path the barriers for formation of products from **3a-2** are quite small compared to the formation of product from either very small or very large angles of attack.

We studied B3LYP/6-31G* classical dynamic trajectories explore the idea of styrene/BH_3 system been also a "hot" reaction. If these trajectories are able form product faster than redistribution of thermal energy, dynamic may explain the experimental selectivity accurately. First, we observed that from dynamic trajectories stated at the complex **3a-2**, not many Markovnikov products are form within 5000 fs. When starting form complex **3a-2**, 78 out of 142 trajectories formed product. From the 78 products

formed 75 trajectories afforded the favored anti-Markovnikov product, which corresponds to a ratio of 96:4. In other words these dynamic trajectories predicted a $\Delta\Delta G^{\ddagger}$ of ~ 1.9 kcal/mol. The result from dynamic trajectories started at the complex represents the reaction selectivity with no excess energy. With no excess energy, as we expected, the selectivity form complex is consistent with transition state theory, though not with experiment, and weighs against recrossing or unknown subtle classical entropy effects as the source of the discrepancy.

When B3LYP/6-31G* classical dynamic trajectories, Figure **3.3**, were started from **3a-5**‡, 33 out of 101 trajectories formed product. From which 27 trajectories afforded the favored anti-Markovnikov product. Meaning, the ratio corresponding to the selectivity of anti-Markovnikov versus Markovnikov products formed form **3a-5**‡ is 82:18, which is equivalent to a $\Delta\Delta G^{\ddagger}$ of ~0.9 kcal/mol. This result now is consistent the fact that trajectories started from points before **3a-5**‡ on the reaction coordinate, thus having excess energy in the area of **3a-5**‡ are consistent with the experimental selectivity.

Table 3.3. Classical Trajectory Studies.

Starting point	Anti-Markovnikov	Markovnikov	Unreactive in 5000 fs	Back to Starting Material within 5000 fs
3a-2	75	3	59	5
3a-5‡	27	6	12	56

From the observations in the trajectories study, Figure **3.3**, we envision the selectivity for the hydroboration of styrene with BH_3 in solution as involving a 'direct-trajectory' stage, with low selectivity, as in the case of propene with BH_3. Also, involving a thermally-equilibrated stage, developing over several picoseconds as the excess energy is transferred to solvent. This last stage should more selective, as evidenced by the results with trajectories starting from **3a-5**‡, but by then the damage is done. However we are the selectivity expected from the last stage is not as large as in the previous case discussed.

H/D Isotope Effect in the Hydroboration of Styrene

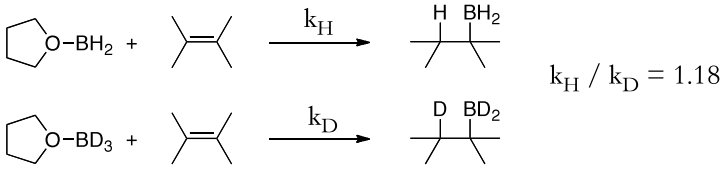
Some unusual experimental observations were described in the previous chapter as clearly contradictory with the conventional mechanistic picture, though it was on agreement with our new mechanistic proposal. The isotope effect determined for the hydroboration of octene was found qualitatively consistent with a low selectivity decided in a dynamically-controlled process. As part of the experimental studies for the hydroboration of styrene we put forward a revision of the isotope effect to determine if the same effect as in the case of propene is observed.

In considering the KIEs for the hydroboration of alkenes by H-B versus D-B bonds of borane, there are two distinct forms of KIEs of interest. The first is an *intermolecular* KIE, reflecting the relative rate for reaction of BH_3 versus BD_3. The second is an *intramolecular* KIE, reflecting the preference for a hydrogen atom versus a deuterium

atom to end up in the product alcohol when both are initially attached to the same boron atom.

The determination of an intermolecular BH_3 / BD_3 KIE cannot be performed by a competition reaction due to a very rapid redistribution of H / D between the borane molecules, so a measurement of the intermolecular KIE would necessarily rely on absolute kinetics. As is the case for the determination of the regioselectivity, the observed reaction of BH_3 or BD_3 with unhindered alkenes is a composite of hydroboration by the parent borane and hydroboration by alkylboranes and dialkylboranes. Sterically unhindered alkylboranes are somewhat more reactive in the hydroboration of simple alkenes than BH_3 itself, and while in principle the BH_3-mediated hydroboration could be observed discretely using a large excess of BH_3, this has not proven practical. Pasto and coworkers were able to determine the intermolecular BH_3 / BD_3 KIE by absolute kinetics in the special-case hydroboration of tetramethylethylene, taking advantage of the much lower reactivity of the hindered thexylborane product. For this reaction, Pasto observed a k_H/k_D of 1.18. While there is some reason to question the precision of this measurement, the intermolecular BH_3 / BD_3 KIE is certainly small.

Scheme 3.4



Intramolecular KIEs are normally straightforwardly measured in competition reactions by an examination of the isotopic distribution in the product, but there are two special complications applicable to hydroborations with BH_3. The first complication is that some portion of the product is unavoidably produced by hydroboration with alkylboranes and dialkylboranes, and the KIE for these alternative reactions need not be the same as that for hydroboration by BH_3. The isotopic distribution in the product will reflect a weighted average of the isotopic results for the contributing processes. To minimize this problem, the reactions here employed a three-fold excess of borane. This does not eliminate the contribution of hydroboration by alkylboranes and dialkylboranes, but the contribution of the BH_3 reaction to the overall result, based on kinetic modeling, is ≈73%. It will be seen that the observed composite KIEs are interpretable despite this complication. The second complication is that a hydroboration by partially deuterated borane consists of hydroborations by four isotopologues: BH_3, BH_2D, BHD_2, and BD_3. When BH_3 and BD_3 are carrying out the hydroboration, there is no direct intramolecular competition, and when BH_2D and BHD_2 are carrying out the hydroboration the intramolecular competition is biased toward the major isotope present. It is straightforward to allow for the four contributing reactions mathematically, and the algebra associated with this process.

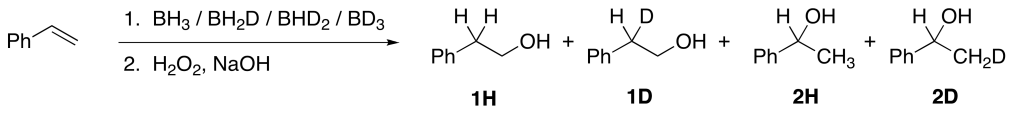
An explanation of the allowance for reactions of four isotopologues BH_3, BH_2D, BHD_2, and BD_3 in calculating the intramolecular isotope effect. For a 1 : 1 ratio of H to D in a sample of borane, it was assumed that the isotopes were statistically distributed at equilibrium. With the assumption, the ratio of BH_3 : BH_2D : BHD_2 : BD_3 would be 1 : 3

: 3 : 1. In a non-Curtin-Hammett situation in which a rate-limiting step committing a molecule of borane to reaction (calculationally, formation of a borane-alkene complex) precedes a product-determining step that decides whether H or D ends up in the product alcohol, 12.5% of the reaction would result from BH_3, 37.5% of the reaction would result from BH_2D, 12.5% of the reaction would result from BHD_2, and 12.5% of the reaction would result from BD_3. For an intramolecular isotope effect k_H/k_D, the relative amount of product from reaction of an H would be 0.125 (from BH_3) + 0.375 x (2 / (2 + $1/(k_H/k_D)$)) (from BH_2D) + 0.375 x (1 / (1 + $2/(k_H/k_D)$)) (from BHD_2). The relative amount of product from reaction of a D would be 0.125 (from BD_3) + 0.375 x (($(1/(k_H/k_D))$ / (2 + $1/(k_H/k_D)$)) (from BH_2D) + 0.375 x ($2/(k_H/k_D)$ / (1 + $2/(k_H/k_D)$)) (from BHD_2). As an example, if the intramolecular isotope effect k_H/k_D were 3, the H product would be 0.125 + 0.3214 + 0.225 and the D product would be 0.125 + 0.0536 + 0.15, and the H/D ratio would be 2.04.

In the event, the intramolecular KIEs for hydroborations were measured in several different ways. Some of the methods employed were intrinsically imprecise and served only to verify the approximate magnitude of the KIE.

As discussed above, the hydroboration of styrene produces a mixture of regioisomeric anti-Markovnikov and Markovnikov products. When partially deuterated borane is employed, the four possible products would be **1H**, **1D**, **2H**, and **2D**. To determine the intramolecular KIEs in these reactions, we first needed to determine the ratios **1H** versus **1D** and **2H** versus **2D** products when using excess borane, relative to the ratio of H versus D in the starting borane.

Scheme 3.5



The most satisfactory method for determining these ratios took advantage of the NMR isotope effect on the chemical shift for protons when there is a geminal deuterium. The benzylic hydrogens in **1H** exhibit a triplet at δ 2.84, while the methyl group in **2H** exhibits a doublet at δ 1.47. The normal isotope effect on the chemical shift for aliphatic protons moves the signals for the deuterated materials **1D** and **2D** to a lower frequency by 0.017 ppm.[86] As shown in Figure **3.4**, this leads to a partial resolution of the signals for deuterated versus non-deuterated materials in both the anti-Markovnikov and Markovnikov products. The relative amounts of the deuterated versus non-deuterated molecules can be determined from the integration of the resolved signals at each end of the pattern. The error resulting from this integration process was minimized by using isotopic calibration standards, using identical baseline and phasing adjustments and integration procedures for the standards (prepared using excess styrene so that the borane reacted to completion and no isotopic fractionation occurs) and the samples (prepared using the same stock solution of borane but using a three-fold excess of borane so that isotopic fractionation can occur).

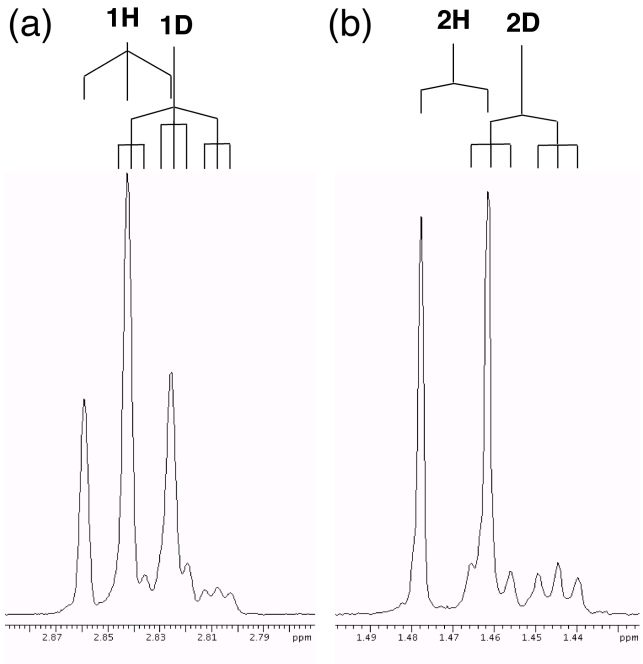


Figure 3.4.. (a) Splitting pattern for the benzylic methylene group of anti-Markovnikov product derived from hydroboration of styrene with partially deuterated borane. (b) Spliting pattern for the methyl group of Markovnikov product derived from hydroboration of styrene with partially deuterated borane. Due to the isotope effect on the chemical shift, the labeled and unlabeled patterns are partially resolved. The ratios of **1H** : **1D** and **2H** : **2D** were based on integrations of the leftmost singlet in each pattern versus the rightmost 1:1:1 triplet, calibrated versus a standard.

In three measurements, the ratios of **1H** : **1D** in the sample versus the **1H** : **1D** in the standard were 1.03, 1.03, and 1.00. As discussed above, these raw values must be corrected to allow for the complication of the four isotopologues BH_3, BH_2D, BHD_2, and BD_3 being involved; when this is done the intramolecular isotope effects are 1.05, 1.05, and 1.00.[87] These numbers in turn reflect a weighted average of the isotope effects for hydroboration by borane, alkylborane, and dialkylborane. With the minimal assumption that the k_H/k_D for hydroboration by alkylborane and dialkylborane is not less than unity,

the intramolecular isotope effect for hydroboration by borane would not be greater than 1.1. This is not consistent with a normal primary H/D isotope effect.

In two measurements, the ratios of **2H** : **2D** in the sample versus the **2H** : **2D** in the standard were 0.98 and 0.94. After correction, the measured intramolecular isotope effects would be 0.97 and 0.91. The precision of these measurements is not sufficient to conclude that the intramolecular isotope effect is less than unity, but the results are again not consistent with a normal primary H/D isotope effect.

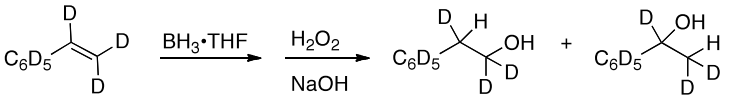
An alternative measure of the isotope effect in the formation of **D** can be garnered from the integration of combined **1H**- **1D** benzylic signals versus their CH_2O signal at δ 3.83. This measurement is intrinsically less precise; a 1 : 1 ratio of **1H** : **1D** leads to a 1.5 : 2 ratio of integrations for the benzylic versus CH_2O signals, while a 2:1 ratio of **1H** : **1D** would only change the benzylic : CH_2O ratio to 1.67 : 1. In three measurements obtained in this way, the ratios of **1H** : **1D** in the sample versus the **1H** : **1D** in the standard were 1.23, 1.07, and 0.99. Though much less precise, these results reinforce the observation that the isotope effect is small.

Once again we can see that because k_H/k_T should exceed k_H/k_D by only a limited extent [74-75]the Pasto isotope effect and the isotope effect here are inconsistent. The origin of this discrepancy is unknown, but the isotope effect determined here is qualitatively consistent with a low selectivity decided in a dynamically-controlled process.

Temperature Effect on the Selectivity

A new unusual observation in the hydroboration of propene-d_6 is that the regioselectivity is surprisingly temperature-insensitive. We decided compare this with the temperature effect on the regioselectivity of this case. The experimental in this case was had a slight difference, the choice of temperature. For the case of propene-d_6, we were not able to obtain reliable results for the reaction below 0 °C due to volatility, however nice reproducible results were obtained at higher temperatures. For the hydroboration of styrene-d_8, since there are no issues with volatility, it was possible to lower the temperature to determine the regioselectivity; opposite to propene-d_6 the trouble was to get a clean ratio at higher temperatures. Finally, the hydroboration of styrene-d_8 at -28, 0, 22 and 70 °C afforded 17.4, 21.3, 23 and 26% Markovnikov addition, respectively (See Table 3.4 below). This corresponds to a $\Delta\Delta H^{\ddagger}$ of only 0.8 kcal/mol. This is yet another observation that support the mechanistic description here.

Table 3.4. Temperature effect on the product regioselectivity in the hydroboration of styrene with BH_3



Temperature (°C)	% A	% B	$\Delta\Delta G^{\ddagger}$ (kcal/mol)
-28	17.4	82.6	0.76
0	21.3	78.7	0.71
22	23	77	0.71
70	26	74	0.71

In conclusion, current understanding of selectivity in ordinary chemical reactions assumes the applicability of the transition state theory model of reactivity. It has been found, in the case of the hydroboration of styrene, transition state theory was inappropriately applied. G3B3 calculations predict too large of an energy difference between competitive transition structures to account for the experimentally observed product ratio. Considering calculational errors, tunneling, and entropy effects does not account for the discrepancy. However, trajectories started from the enthalpic association barrier found following the steepest-descent path, better predicts the experimental selectivity. This represents another example in which transition state theory is proven to be inapplicable when the branching deciding the selectivity located after the rate-limiting transition structure. In this well-know reaction, consideration of dynamic trajectories is essential for explaining the experimental outcome.

CHAPTER IV

DYNAMICS AND SELECTIVITY IN THE HYDROBORATION OF INTERNAL DISUBSTITUTED AND TRISUBSTITUTED ALKENES

Introduction

From our results of previous chapters it is fascinating to consider the applicability to consider the dynamic effect idea for other alkene hydroborations. However, this could be an arduous task. To explore the impact of dynamics on more highly substituted alkenes we selected a representative group of disubstituted and trisubstituted alkenes.

The regioselectivity of hydroborations of highly substituted alkenes compared to that of less substituted alkenes has been of interest since the discovery of hydroboration. The reactivity and selectivity for hydroborations of highly substituted alkenes are generally explained using sterics as the predominate factor. In more detail, the kinetic selectivity in hydroboration is viewed as the result of the two differing transition state barriers that lead to the alternative products. This has been applied without considering the fact that an exothermic association process with a free energy barrier might be involved and this association free energy barrier could be the rate-limiting step. The combination of the rate limiting association and the potential role of dynamic effects provides a new mechanistic interpretation of experimental observations of experimental reactivities and selectivities with highly substitutive alkenes.

These remarks leave some essential questions: Is there a discrepancy between the experimental selectivity and transition state theory for the hydroboration of highly

substituted olefins with BH_3? If so, do dynamic trajectories account for the observed selectivity?

To test this, high level calculations were used to predict the $\Delta\Delta G^{\ddagger}$ from the two transition states leading to the regioisomeric products. This let us know if the experimental ratio is what would be expected by transition state theory. An accurate computational approach is necessary. From previous examples we examined a large combination of *ab initio* or DFT methods and basis sets for their ability to model the potential energy surface for addition of BH_3 to propene, as judged by comparison with CCSD(T)/aug-cc-pvtz energies.[me] The B3LYP/6-31G* calculations performed the best among DFT functionals / basis sets tested for geometry optimizations and trajectory calculations. This means that B3LYP/6-31G* would be a good choice for trajectory calculations and it also means that composite methods that are built on B3YLP geometries should be good for determining energies. This is what was found for accurate energies, G3B3 energies performed very well matching CCSD(T)/aug-cc-pvtz with in 0.1 Kcal/mol. For this reason, G3B3 calculations were selected for the study of the larger hydroboration reactions.

Theoretical Pathway in the Reaction Model of the Hydroboration of Trans-2-butene with BH_3

The kinetics of hydroboration of trans-2-butene were studied by Brown in 1984.[88] For these studies he started with the borinane dimer (R_2HBBHR_2). He found that most alkenes showed three-halves-order rate behavior. This led him to conclude that the

monomer-dimer dissociation equilibrium is fast and that the rate-limiting step is the reaction of the monomer with the alkene as seen in the previous case of 9-BBN. Brown considered that this mechanism of hydroboration with dimeric monofunctional boranes was general. Brown also observed that the hydroboration of *cis*-2-butene is faster than the corresponding reaction with *trans*-2-butene. The rationalization for the difference on the reaction rate, 5.40 for cis-2-butene and 3.55 for trans-2-butene, is that there is relief of strain in the transition state for hydroboration of the *cis*-alkene. This is notable because it is the hydroboration transition state and not an association transition state is supplying the rationalization for the observation.

When chiral dialkylboranes are used for the hydroboration of disubstituted alkenes, there can asymmetric induction in the generation in the product alcohol. *Trans*-2-butene is a prochiral alkene that was used to determine the potential for asymmetric hydroboration with a variety of enantiomerically pure boranes.

The historical importance of hydroborations of trans-2-butene makes it an important subject for our study of the potential role of dynamics in the selectivity of hydroboration reactions. In the simple hydroboration of *trans*-2-butene no regioselectivity was involved. Our purpose was to explore this prototypical reaction to the reaction energetics if the free energy barrier for association as opposed to the actual hydroboration step is rate-limiting.

Table 4.1. Enthalpies and free energies for calculated structures in the hydroboration of trans-2-butene with BH_3.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4a-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
4a-4‡	$\Delta G^{\ddagger} = 5.2$ $\Delta H^{\ddagger} = -2.3$	$\Delta G^{\ddagger} = 6.1$ $\Delta H^{\ddagger} = -2.2$	$\Delta G^{\ddagger} = 6.4$ $\Delta H^{\ddagger} = -1.4$
4a-2	$\Delta G = -1.5$ $\Delta H = -11.7$	$\Delta G = 1.9$ $\Delta H = -11.1$	$\Delta G = 3.4$ $\Delta H = -9.6$
4a-3‡	$\Delta G^{\ddagger} = -1.0$ $\Delta H^{\ddagger} = -10.8$	$\Delta G^{\ddagger} = 4.6$ $\Delta H^{\ddagger} = -9.2$	$\Delta G^{\ddagger} = 5.5$ $\Delta H^{\ddagger} = -8.2$
4a-5	$\Delta G = -15.8$ $\Delta H = -26.1$	$\Delta G = -12.7$ $\Delta H = -26.9$	$\Delta G = -11.3$ $\Delta H = -12.9$

The energies are relative to the starting materials and is expressed in Kcal/mol. The enthalpies and free energies are calculated at 25 deg. C.

In gas-phase B3LYP with both 6-31+G** or 6-31G* in these calculation's basis set, we located the π-complex **4a-2** and hydroboration transition structure **4a-3**‡ for the hydroboration of trans-2-butene with BH_3 were located. For the structures found the relative energetics were determine with G3B3, B3LYP/6-31G* and B3LYP/6-31+G**

calculations. The complete list of the calculated enthalpies and free energies for each method and structure are shown in Table **4.1** relative to the separate starting materials.

Our discussion will focus on the most reliable G3B3 energies. The calculated enthalpic barrier between the complex and the product formation transition state is only 0.9 kcal/mol. The formation of complex **4a-2** from BH_3 / *trans*-2-butene is enthalpically barrierless. However, such association reactions always involve an entropic barrier. Within variational transition state theory, the variational transition state for such a process is when the free energy reaches a maximum along the free energy path. We proceeded to search for this variational transition state.

The starting point for the location of variational transition state **4-a4**‡ was the optimized structure found in a scan of positions with BH_3 and *trans*-2-butene centroids separated by 5 Å. From this structure, a steepest-descent path in mass-weighted coordinates was followed. The steepest-descent path was obtained using a modified version of PROGDYN[83,84], in which no momentum is given to nuclei and very small steps (< 0.00025 Å) are used, varying the size of the steps continually to avoid oscillations. This approach has the problem of being extremely slow compared to other approaches, but it has the virtue of being extremely reliable. The steepest decent path was obtained using a modified version of PROGDYN as described in previous chapters. For every 40th structure along the steepest-descent path, the free energy was calculated the variational transition state structure 4a-4‡ was identified the free energy maximum along this path that exhibited greater than one imaginary frequency. Having the energetics we can generate a reaction coordinate graph stopping when it finds a

minimum, in this case complex **4a-2**. From the graph we can easily find any barrier is present between starting materials and complex.

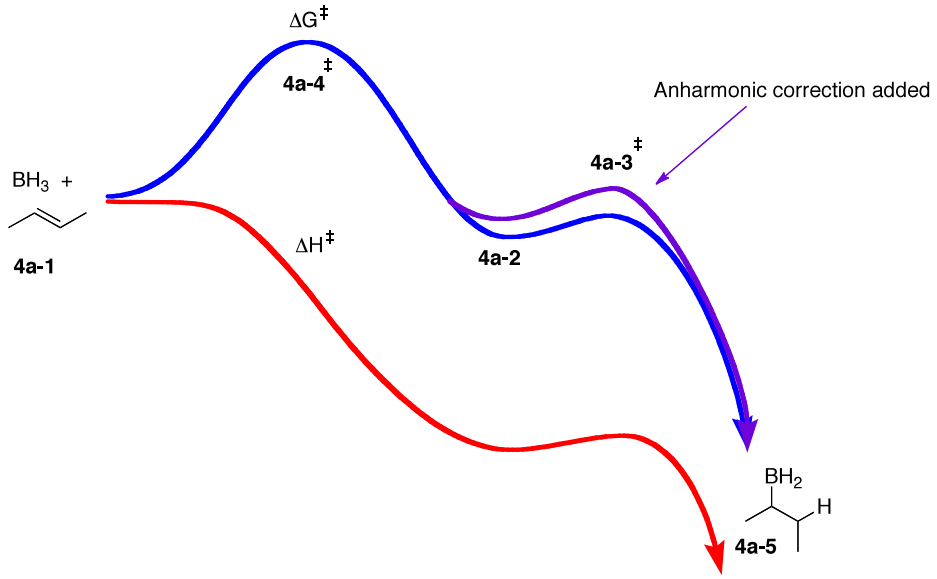


Figure 4.1. Enthalpy and free energy reaction coordinate diagrams for the hydroboration with trans-2-butene with BH_3.

For the hydroboration of BH_3 / *trans*-2-butene we found the variational transition structure **4a-4**‡. The complex 4a-2 is enthalpically 11.7 kcal/mol below the separate starting materials and it is 9.4 kcal/mol below the variational transition state 4a-4‡. As a result the complex 4a-2 is formed with significant excess energy. The barrier for formation of product 4a-5 from 4a-2 is only 0.9 kcal/mol so the excess energy present in 4a-2 is much more than is needed to overcome the barrier for product formation. As a result, we can conclude that, significant excess energy is thus available from the formation of **4a-2**, and the barrier for formation of product **4a-5** from **4a-2** is small. As was the case for propene, the formation of product may be faster than a thermal

equilibration with the solvent. The reaction coordinate diagram for the reaction is shown in Figure **4.1**.

As in other cases we explored the effect of an anharmonic correction on the energetics. The anharmonic corrections change the energies modestly and interestingly bring the free energy for reaction from the complex over the product forming transition state down somewhat. This makes the prospects for dynamic effect in these reactions even greater. The free energy barrier starts out at about 2.5 kcal/mol and after inclusion of the anharmonic correction the free energy barrier goes down to about 0.8 kcal/mol. Of course in the case of trans-2-butene there is no regioselectivity to be affected by a dynamic affect in the reaction, but it may be of interest in future studies to determine if an isotope effect can be observed in this reaction that would be the result of a dynamic effect.

Table 4.2. Calculated free energy after anharmonic adjustment for the structures located.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4a-2	$\Delta G = -1.0$	$\Delta G = 2.4$	$\Delta G = 3.9$
4a-3‡	$\Delta G^{\ddagger} = 0.2$	$\Delta G^{\ddagger} = 3.8$	$\Delta G^{\ddagger} = 4.8$

According to methods/basis sets; G3B3, B3LYP/6-31G* and B3LYP/6-31+G** calculations, they are relative to the starting material and expressed in kcal/mol.

Table **4.2** lists the corrected energies for the transition structure **4a-3**‡ and complex **4a-2**, form this analysis we can observe that barrier for the formation of the product is 1.2 kcal/mol instead of the 1.4 kcal/mol. From the analysis we also determined that the difference in energy between the variational transition state **4a-4**‡ and the complex **4a-2**, was 6.2 kcal/mol compared to the 6.7 kcal/mol predicted without corrections.

To summarize, from the theoretical reevaluation of the mechanism of hydroboration of trans-2-butene, we find the reaction precedes though an exothermic association process and that there is no enthalpic barrier for this association. The entropic barrier leads this association to be the rate-limiting step in the reaction. The low energy of the complex compared to separate starting materials will mean that there is excess energy in the complex on its formation and the low energy of the barrier going on from the complex suggest that the rate of product formation from the complex with its excess energy will be subject to a dynamic effect

Intramolecular H/D Isotope Effect For The Hydroboration of Tetramethylethylene with BH_3

In an older mechanistic study Pasto studied a series of isotope effects for hydroboration of tetramethylethylene with BH_3 and included intermolecular hydrogen-deuterium isotope effects on the absolute rate, intramolecular hydrogen-tritium isotope effects on product formation, and competition $^{10}B/^{11}B$ kinetic isotope effects. The hydrogen-deuterium KIE on the absolute rate observed by Pasto was 1.18. Pasto

interpreted this value as a superposition of a primary and secondary isotope effect. Pasto expected that a primary isotope effect would have a value greater than unity while a secondary isotope will be less than unity.[89] Because the 1.18 value was lowered by the assumed significantly inverse secondary isotope effect, Pasto did not recognize that the unusual character of the small isotope effect for a reaction in which hydrogen is being transferred. Normally if hydrogen is transferred during a rate limiting step the hydrogen-deuterium isotope effect would be greater than 2. It should be recognized at the time, the ideas related with an association transition state being a variational transition state and rate limiting had not been developed. Pasto could not have easily interpreted his small isotope effect in any other way. Pasto observed an intramolecular isotope effect on H/T of 3.3, this was interpreted of reflecting the normal isotope effect for the hydroboration step without any inference from an inverse isotope effect. Pasto then noted that after an allowance between hydrogen and tritium the 3.3 agrees reasonably well with KIEs observed with 1-hecene and styrene in reactions of these alkenes with a monochloroborane in THF.[89]

The hydrogen-tritium isotope effects are intramolecular isotope effects that decide rather the product contains a hydrogen or tritium. In general, intramolecular isotope effects reflect the first irreversibly unsymmetrical step in a mechanism and this is not the rate-limiting step. The intramolecular isotope effect observed by Pasto decreased with increasing substitution on the double bond as well as with increasing substitution on the boron. Pasto interpreted these isotope effects as consistent with the decrease C-H bond formation and a B_H bond breaking in the transition state due to steric factors. He

also concluded that the observed isotope effect is not consistent with a secondary isotope effect arising from the formation of a π-complex between the borane and alkene in the rate-determining step.

The isotope effect of $^{10}B/^{11}B$ was measured and Pasto deduced that an intermolecular competition between H and T was present and resembles the isotope effect for the product-determining step. The results Pasto obtained led him to believe that the isotope effect increased very slightly with increasing substitution on the double bond. He thought that this is consistent with an increase in the bonding interaction between the boron and carbon to the increase in the π-electron density of the double bond. Pasto concluded that the electronic effect offset the steric effect that would otherwise help to decrease the isotope effect as the degree of substitution on the double bond increased. It was thought the combination of the hydrogen-tritium and $^{10}B/^{11}B$ isotope effects suggests that C-H and C-B bond formation and B-H and C=C bond breaking occur in concert during the formation of a four-centered transition state. This interpretation is strained by the necessity by postulating a large inverse isotope effect that counterbalances the normal isotope an enormous in order to get to Pasto's absolute effect of 1.1. We will see in the work described the isotope effects become more consistent with the new experimental KIE's that we will present.

Scheme 4.1.

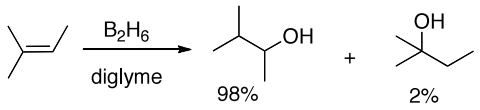
The hydroboration of tetramethylethylene on a 1:1 molar basis to afford thexylborane is a commonly employed synthetic procedure. After oxidation to afford tetramethylethylene, the ratio of **3H** to **3D** was determined in two ways. The first way employed ^{1}H NMR, taking advantage of a vicinal isotope effect of deuterium on the chemical shift of the isopropyl methyls of the product from the hydroboration of tetramethylethylene, leading to resolution of high-frequency signal of the isopropyl group doublet of **3H**. The corresponding signal for **3D** is unresolved but its amount was inferred by subtracting out the expected integration for **3H** from the integral of the overlapping signals. A more satisfactory direct measurement was obtained from ^{13}C NMR analysis of the product from the hydroboration of tetramethylethylene. Employing conditions suitable for ^{13}C NMR integration,[48] the fully resolved singlet and triplet signals for the methene carbons of **3H** and **3D**, respectively, could be integrated to determine the ratio of the isotopologs. From five measurements (three by the ^{1}H NMR process, two by the ^{13}C NMR process, the isotope effect was 1.24 ± 0.06. From the five measurements of the ratio of **3H** to **3D** gave values 0.635, 0.625, 0.611, 0.616, and 0.630. This leads to an **3H** : **3D** ratio of 0.624 ± 0.012. By taking the ratio to that determined for the stock solution (0.502 ± 0.024) and propagating the errors in a standard way, the isotope effect was 1.24 ± 0.06. This isotope effect is somewhat larger than what we observe in the hydroborations of 1-octene, styrene, and 2-methyl-2butene, but it is still a quit small isotope effect; within the conventional interpretation of isotope effects of greater than 2. At 1.24 there is some suggestion of hydrogen versus deuterium making some difference, but not a great amount of difference. It seems possible that this

could result from an reaction in which the selectivity was determined in a combination affects that we have proposed for the hydroboration of propene. For that proportion of the reaction that is governed by transition state theory, the isotope effect should be relatively large and that would tend to raise the overall k_H/k_D for a portion of the isotope effect that arose from direct trajectories, one might expect the isotope might be small. There then could be in vision to that the isotope effect in the case of tetramethylethylene results from a combination of these two possibilities. This interpretation suggests that with tetramethylethylene there is a larger portion of products formed by a process that is approximately controlled by transition state theory. Then is the case in the hydroborations of the other alkenes. Nonetheless the isotope effect is too small for the conventional mechanism to be the predominate pathway.

Isotope Effects, Dynamics, and the Nature of Selectivity in the Hydroboration of 2-Methyl-2-Butene with BH_3

The regioselectivity for the hydroboration of 2-methyl-2-butene is notably greater than that observed with a monosubstituted alkene. Brown attributed this selectivity to a powerful directive effect of sterics at the transition state.[14]

Scheme 4.2.

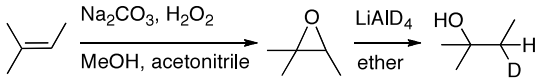


Brown explored the rate and stoichiometry for the hydroboration of 2-methyl-2butene with BH_3 in detail. This reaction stops at an earlier stage than the hydroboration of monosubstituted alkenes. The trialkylborane is formed at a very low rate and Brown reported a procedure for the selective synthesis for the disiamylborane. Such dialkylboranes are not obtainable in hydroborations of monosubstituted alkenes. The synthetic value of disiamylborane is that it is a highly selective hydroborating agent. According to Brown's synthetic study, once Disiamylborane is formed the third hydroboration to form tridisiamylborane is only 40% complete after 24 h. The regioselectivity observed under normal circumstances in the hydroboration of 2-methy-2-butene with BH_3 is a composite of only two steps hydroboration by and hydroboration by RBH_2. In our studies, we have measured the selectivity for the BH_3 reaction by the approach of using a very large excess of BH_3. This approach is designed to minimize the contribution designed to minimize the contribution of hydroborations by the monoalkylborane to the selectivity.

The process used to examine the regioselectivity of hydroboration of monosubstituted alkenes that was described in a previous chapter runs into some problems in the case of 2-methyl-2-butene and was modified. One problem explained previously was that small amounts of impurities in the BH_3-THF, for example from THF decomposition, could interfere with the analysis. This problem is a greater determent in the study of the hydroboration of 2-methyl-2-butene since the amount of the minor regioisomers obtained in the reaction is very small. In addition, unlike in the case of the monosubstituted alkene, the study of the regioselectivity for the hydroboration of 2-

methyl-2butene cannot take advantage of deuterated starting materials for the direct observation for the selectivity. A disappointing attempt to clearly identify the chemical shifts of the products by ^{2}H NMR was investigated by synthesizing the Markovnikov alcohol though a different route. The volatile 2,2,3-trimethyloxirane was successfully prepared.[90] Subsequently, the crude product with some solvent traces was put forward for the ring opening reaction with $LiAlD_4$ to obtain the desired product as determined by ^{1}H NMR.

Scheme 4.3.

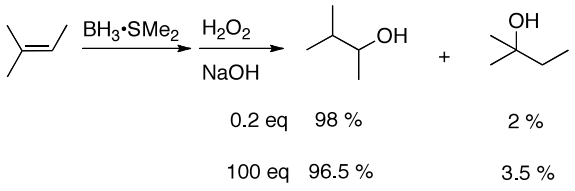


Despite the fact that the product was obtained, it was not completely pure and the purification process would have been time consuming due to the volatility of the product. At last, not a clear chemical shift was obtained. In spite of this, by this point we had completely distinctive approach in mind to solve the challenge.

The use of a different ligand (BH_3•SMe_2 as opposed to THF) is a complication because some papers have proposed that BH_3 is directly transferred from the ligand.[67] As we have noted previously, the weight of evidence in the literature favors a more of an SN1 mechanism in which the BH_3 is free prior to reacting with the alkene. It is notable that small regioselectivity differences can be observed in hydroboration depending on the particular borane ligand being used. However, such regioselectivity differences can

potentially arise from the effect of varying contributions from reactions of BH_3 versus alkyl or dialkyl boranes.

Scheme 4.4



In our study of the hydroboration of 2-methyl-2-butene 2% of the regioisomer was obtained when a deffiecency of borane was employed (0.2 eq), but the selectivity went down when 100 eq of borane were added with a reaction affordding 3.5% of the minor regioisomer. It is uncertain weather a 100 eq is sufficient to reach a limiting ratio of this reaction. The $\Delta\Delta G^{\ddagger}$ corresponding a 96.5 to a 3.5 ratio is 2.0 kcal/mol. A complication in the 2-methyl-2-butene reaction was that the product ratios varied slightly depending upon the exact reaction condition and exhibited some traces of products attributed to isomerization. Accordinly the reaction had to be done with more care. To attain reliable results we took the approach of limiting the reaction time to five hours and oxidizing the reaction mixture only after lowering the temperature to 30 °C with a very slow addition of the oxidant to avoid overheating. It appeared that the use of more than 2 eq. of alkene relative to borane promoted isomerization so we were careul to limit of excess borane to no more than 2 eq.

As was mentioned, 2-methyl-2-butene forms disiamylborane rapidly and only slowly starts to form trisiamylborane. Brown's experiment, which was performed with the purpose of learning about the rate of these conversions used 0.3 equivalents of borane relative to alkene. The 98:2 anti-Markovnikov to Markovnikov selectivity reported was for a reaction using 1.2 M of 2-methyl-2-butene and 0.6 M of borane with a reaction time of 9 hours. We examined carefully the hydroboration using 0.3 equivalents of borane relative to alkene to determine the highest selectivity observed corresponding the addition of the olefin to the borane to form trisiamylborane. After the oxidation toluene-d^8 was added to extract the product and the resulting solution was analyzed by ^{1}H-NMR. This lead to an impure mixture, not just the two alcohols expected, Scheme 4.4. After considering the possibility of isomerization, we reanalyzed the spectra to see what alcohol isomers could be recognized. The estimate for the major product obtained versus the other isomers in the specific case, in which the reaction had been allowed to continue for three days, was calculated roughly to be 20:80 percent.

Interestingly, isomerization was also observed in cases where excess borane was also used when the reactions were left for long periods of time. When 44 equivalents of borane was used and the reaction was allowed to continue for two and a half weeks the ^{1}H NMR spectra of the product exhibited isomerized alcohols. The amount of isomerized alcohol was estimated by taking all of the peaks overlapped in the range of δ 0.8 – 0.95 ppm and assuming this range corresponded to the total amount of alcohols, then subtracting the portion that was attributable to the normal anti-Markovnikov product based on the integration of the doublet at ~ δ 1.15 ppm. An approximately

30:70 ratio of the anti-Markovnikov product to other isomers was obtained. In spite of these complications, we were able to estimate the anti-Markovnikov to Markovnikov selectivity for reactions, but yet we were able to determine the anti-Markovnikov to Markovnikov selectivity for reactions with negligible isomerization. , This observation was why we concluded that the δ 0.8 – 0.95 ppm peak belongs to the isomers only.

Finally, for the reaction of 100 equivalents of borane relative to the amount of alkene, after two and a half weeks we found less isomerization compare to the same reaction with 44 equivalents. The approximate ratio calculated for this reaction was 66:34, this approximation was establish by integrating the peaks identified for some of the isomers found between δ 3 – 4 ppm.

Our next step was to see if the observed regioselectivity of 96.5:3.5 was consistent with our predictions based on transition state theory. As in previous cases, the hydroboration of 2-methyl-2-butene with BH_3 was investigated using G3B3, B3LYP/6-31G* and B3LYP/6-31+G** calculations. A summary of the energies obtained can be found in Table **4.3**. Two hydroboration transition states were located **4c-3**‡, which leads to the anti-Markovnikov product and **4c-4**‡ which leads to the Markovnikov product. The G3B3 calculation predicted a free energy difference between these structures of 2.68 kcal/mol. The selectivity expected from the free energy difference would be 99:1, which is significantly greater from what we observed experimentally. However, the energy difference in this case is a lot smaller than what was observed with propene. That is the 2.68 kcal/mol that is predicted calculationally may be compared with an experimental difference based on the 96.5:3.5 ratio of 2.0

Table 4.3. Enthalpies and free energies for calculated structures for the hydroboration of BH_3 with 2-methyl-2-butene.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4c-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
4c-5‡	$\Delta G^{\ddagger} = 5.0$ $\Delta H^{\ddagger} = -3.6$	$\Delta G^{\ddagger} = -6.3$ $\Delta H^{\ddagger} = -2.4$	$\Delta G^{\ddagger} = 6.6$ $\Delta H^{\ddagger} = -1.8$
4c-2	$\Delta G = -3.4$ $\Delta H = -13.4$	$\Delta G = 1.4$ $\Delta H = -10.9$	$\Delta G = 2.4$ $\Delta H = -9.8$
4c-3‡	$\Delta G^{\ddagger} = -0.4$ $\Delta H^{\ddagger} = -12.6$	$\Delta G^{\ddagger} = 5.2$ $\Delta H^{\ddagger} = -8.9$	$\Delta G^{\ddagger} = 5.8$ $\Delta H^{\ddagger} = -8.4$
4c-4‡	$\Delta G^{\ddagger} = 2.2$ $\Delta H^{\ddagger} = -10.1$	$\Delta G^{\ddagger} = 7.7$ $\Delta H^{\ddagger} = -6.6$	$\Delta G^{\ddagger} = 8.5$ $\Delta H^{\ddagger} = -5.8$
4c-6	$\Delta G = -14.7$ $\Delta H = -25.6$	$\Delta G = -9.8$ $\Delta H = -24.2$	$\Delta G = -8.9$ $\Delta H = -23.4$
4c-7	$\Delta G = -14.7$ $\Delta H = -25.7$	$\Delta G = -9.1$ $\Delta H = -23.7$	$\Delta G = -8.0$ $\Delta H = -22.7$

According to methods/basis set G3B3, B3LYP/6-31G* and B3LYP/6-31+G** calculations, they are relative to the starting material and expressed in kcal/mol.

kcal/mol. A discrepancy of 0.6 kcal/mol is significant, but is intransigently less convincing than the greater than 1.2 kcal/mol discrepancy seen with monosubstituted alkenes. This analysis has not yet considered any correction for anharmonicity.

Table 4.4. Free energy predicted after anharmonic adjustment for the structures located for the system BH_3/2-methyl-2-butene.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4c-2	$\Delta G = -3.0$	$\Delta G = 1.8$	$\Delta G = 2.8$
4c-3‡	$\Delta G^{\ddagger} = -0.7$	$\Delta G^{\ddagger} = 4.9$	$\Delta G^{\ddagger} = 5.5$
4c-4‡	$\Delta G^{\ddagger} = 1.2$	$\Delta G^{\ddagger} = 6.7$	$\Delta G^{\ddagger} = 7.5$

According to methods/basis sets; G3B3, B3LYP/6-31G* and B3LYP/6-31+G** calculations, they are relative to the starting material and expressed in kcal/mol.

As in previous cases, an anharmonic correction was obtained for the energies for the complex **4c-2**‡ the competitive energy states **4c-2**‡ and **4c-4**$^{\ddagger t}$. These corrections are summarized in Table **4.4**. The calculated $\Delta\Delta G^{\ddagger}$ with these corrections is reduced to 1.8 kcal/mol. This matches very closely with what would be calculated based on a transition state theory analysis of the experimental selectivity. As a result, the experimental selectivity provided no evidence for the importance of a dynamic effect for this reaction. It does not exclude the importance of the dynamic effect, as it is perfectly possible for

dynamic selectivity and for transition state theory to be similar. Another observation in this reaction, the kinetic isotope effect will favor the importance of dynamic effects.

The anharmonic correction of the energies found ought to provide a more accurate approximation, which represent a significantly more accurate comparison of the experimental and ratio calculated for such relatively small energy differences. The estimated $\Delta\Delta G^{\ddagger}$ has been corrected to be approximately 2.0 kcal/mol, which better falls in with the difference in energy assuming the applicability of transition state theory. The detailed $\Delta\Delta G^{\ddagger}$ predicted with and without the anharmonic corrections can be found in Table **4.5**.

Table 4.5. Calculated $\Delta\Delta G^{\ddagger}$ for transition states **4c-3**‡ or **4c-4**‡ with and without anharmonic corrections.

Method / Basis Set	No correction	Anharmonic correction
g3b3	$\Delta\Delta G^{\ddagger} = 2.6$	$\Delta\Delta G^{\ddagger} = 1.8$
B3LYP/6-31G*	$\Delta\Delta G^{\ddagger} = 2.5$	$\Delta\Delta G^{\ddagger} = 1.8$
B3LYP/6-31+G**	$\Delta\Delta G^{\ddagger} = 2.7$	$\Delta\Delta G^{\ddagger} = 2.0$

Form the theoretical predictions, there is no enthalpic barrier for the approach of BH_3 to 2-methyl-2-butene. A variational transition state (**4c-5**‡) for the association of the BH_3 with the olefin was located by adaption an adaptation of the "nosaddle" procedure of Truhlar and coworkers. An analogy to the process used for other alkenes, the starting

point before the location of the variational transition point was obtained by optimizing a structure of the BH_3 and 2-methyl-2-butene centroids separated by 5 Å. The steepest-descent path in mass-weighted coordinates was then obtained using PROGDYN.[84] For every fiftieth structure along the path a frequency calculation was performed and the free energy was calculated and the variational transition state was assigned to the maximum and free energy along the path. The free energy barrier for the variational transition state was 5 kcal/mol.

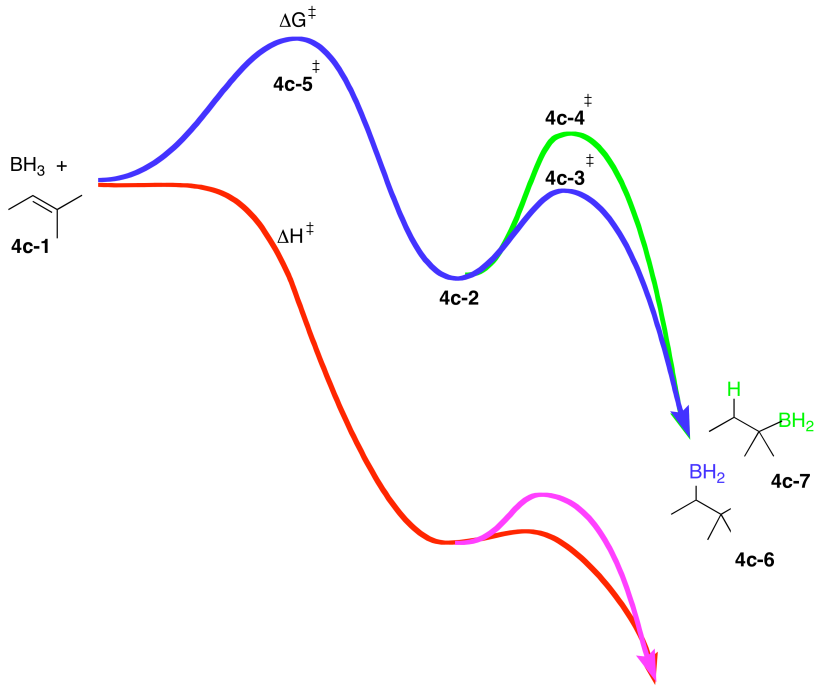


Figure 4.2. Enthalpy and free energy reaction coordinate diagrams for the hydroboration with 2-methyl-2-butene with BH_3.

The enthalpic and free energy coordinates can be seen in Figure **4.2**. A notable feature of this reaction coordinate in comparison with that observed with propene is that the barrier to generate a graph that represents the reaction coordinates for the system,

which ends when it finds the first lowest energy structure, complex **4c-2**. The barrier for the variational transition structure **4c-5**‡ is now located straightforward. The resultant reaction coordinate diagram can be observed in the picture below.

The free energy from passing through the variational transition state **4c-5**‡ is 5.0 kcal/mol. This first barrier is 3.7 kcal/mol higher than the barrier predicted for the Markovnikov transition sate. Relative to the π-complex the barrier is 4.3 kcal/mol for the formation of the Markovnikov product and 1.7 kcal/mol for the formation of the anti-Markovnikov product. This implicates that in spite of the fact that significant excess is available to form the products from the formation of complex **4e-2**, coming down such large magnitude hill, the barrier for the formation of **4c-3**‡ and **4c-4**‡ is somewhat large. In such situation, very few trajectories go directly to products; the largest part of them is faster at thermal equilibration with solvent. The end result is that in these circumstances the transition state theory can get a reasonably accurate selectivity prediction.

Trajectory studies suggest that considerable product would be formed while the π-complex is still hot. When 58 trajectories were started at **4c-2** only 3 afforded product within a 5,000 fs time limit. This rate is consistent with G3B3 predicted free energy barrier of about 3 kcal/mol. None of the trajectories afforded the Markovnikov product, but the low number of trajectories precluded any conclusion from this.. The same outcome is observed for the dynamic trajectories stated at the variational transition structure **4c-5**‡, for which all the products formed where anti-Markovnikov after 5000 fs equilibrations. Nonetheless, the rate of success as forming products was higher.

Of 17 trajectories started at the variational transition structure, **4c-5**‡, eight afforded product. This is a significantly greater proportion then what was seen for trajectories started at the complex. These results suggest that the excess energy that is present when the complex forms from the association of the borane with the alkene would lead to some of the product being formed rapidly.

In summary, the calculated selectivity from transition state theory in comparison from the experimental selectivity provides no evidence for a dynamic effect in this hydroboration. However, the trajectory studies suggest that a substantial amount of product would be formed on a timescale that is faster than thermal equilibration. As a result it is possible that a possible match between transition state theory expected selectivity and the experimental selectivity is fortuitous. We will examine this issue again after a different probe of selectivity in this reaction, that of the kinetic isotope effect.

H/D Isotope Effect in the Hydroboration of 2-Methyl-2-butene

The hydrogen-tritium effect observed by Pasto was 3.01 to 3.25. In two measurements $^{10}B/^{11}B$ isotope effect with 2-methyl-2-butene Pasto observed KIE's 1.044 ± 0.006 and 1.057 ± 0.006. As before these values were taken supporting a four-centered transition state. Other kinetic isotope effect experiments were calculated with and without the inclusion of K_H/K_D on monosubstituted [1-hexene, 9.59-10.00,10.85-11.29; Styrene 10-.00-9.00, 10.44-10.35] and disubstituted [3-Hexene, 6.92, 8.73; 2-Octene, 7.38-8.89; 2-Ethyl-1-hexene, 7.47, 8.99; Propenylbenzene, 7.24, 9.01] with BH_3 as well. All these kinetic isotope experiments were part of the work for which he

generalized, from the hydrogen-tritium and $^{10}B/^{11}B$ isotope effects, that the reaction proceeds through a unsymmetrical four-centered transition with C-H and C-B bond formation occurring in concert with B-H and C=C bond breaking, using as an example the description of the isotope effect for tetramethylethylene. Our isotope effect is not constant with Pasto's, he measured a hydrogen-tritium isotope effect and we measured a hydrogen deuterium isotope effect. The difference that is observed is far outside of any understandable difference due to the isotope effects and there is simply a discrepancy between Pasto's results and ours. As will be seen, we observed isotope effects that do not fit with Pasto's observations.

Although borane will add twice to 2-methyl-2-butene to afford disiamylborane, the second addition is much slower than the first (ref to one of the Pasto papers I believe). As a result, when excess borane is used the isotope effect observed in the reaction should predominantly reflect simple borane addition. This advantage versus terminal alkenes like styrene is counterbalanced by the disadvantage that the B-H bonds of the borane cannot be reacted to completion with the 2-methyl-2-butene, precluding the generation of a direct isotopic calibration standard of the product **5**. Instead, the ratio of H to D in the stock borane solutions used for these reactions was quantified by reacting the solution with excess 1-octene and determining the ratio of the deuterated versus non-deuterated 1-octanol product by integration of the resolved ^{13}C NMR signals of the two materials. The ratio of **4H** to **4D** was then determined directly from the ^{1}H NMR integration of the methene proton of **5** versus the methyl and isopropyl group signals.

It is clear that the K_H/K_D is not consistent with a normal primary H/D isotope effect. For the hydroboration of 2-methyl-2-butene with partially deuterated borane, four measurements of the H : D ratio in the stock solution by the process described gave values 0.480, 0.504, 0.515, and 0.508. The leads to H : D ratio of 0.502 ± 0.024. The six measurements of the ratio of **4H** to **4D** gave values 0.457, 0.485, 0.490, 0.446, 0.465, and 0.464, from three independent reactions. This leads to a **4H** : **4D** ratio of 0.468 ± 0.018. By taking the average of these ratios and propagating the errors in a standard way, the isotope effect was 0.93, and the 95% confidence range, treating each measurement as independent, was ±0.06. Because of the complications in this process, the reliable accuracy of this KIE measurement is unlikely to be better than ±10%. Accordingly, it is not clear that the k_H/k_D is really less than unity, but the isotope effect is small and the results are again not consistent with a normal primary H/D isotope effect.

Not all three independent reactions where prepared with the same ratios of borane to alkene. However, when using either 3 or 0.3 equivalents of borane to alkene, the measurements where analogous. This is due to the fact that the trialkylborane is not likely to be formed.

Scheme 4.5.

4H **4D**

To ensure that the observed isotopic ratio was the result of kinetic rather than thermodynamic process, a control experiment was carried out in which the

hydroboration of 2-methyl-2-butene was first conducted with 3 equiv of BH_3, then 3 equiv of BD_3 was added. After 12 h at 22 °C, the reaction was worked up oxidatively and the **4** was analyzed for deuterium content. None could be detected by ^{13}C NMR.

The small K_H/K_D suggest that a dynamic effect does play a role in the hydroboration 2-methyl-2-butene. The suggestion from this observation is that the math up of transition state predictions theory with observed selectivity is fortitudinous. In an isotope effect the competing possibilities are traveling over the same energy surface and the isotope effect arises from zero point energies and other factors that is normal. It would be unusual for a dynamic control process to mimic the zero point energy factors involved in an isotope effect. Looking at the regioselectivity, a dynamic control process still has to cross-differing heights of barriers in order to get to a completive form of product. Under those circumstances it is easy to envision an accidental agreement of transition state theory with experiment. These ideas suggest that isotope effects may be a more sensitive probe for dynamic effects than product regioselectivities.

Calculated Pathway for the Hydroboration of 1-Methylcyclohexene with BH_3.

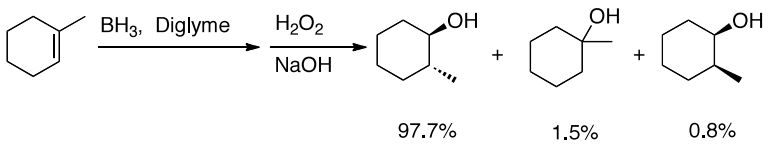
The investigation of the hydroboration of more substituted olefins included the study of cyclic alkenes. Brown's study of cycloalkenes including 1-methylcyclohexene lead to the generalization that hydroboration proceeds through a *cis-anti*-Markovnikov addition of the B-H bond to the alkene. This hydroboration is very selective affording *trans*-2-methylcyclohexanol from the hydroboration of 1-methylcyclohexene. Brown studied relative rates of reactions from various alkenes and found a rate factor 15 for 1-

methylcyclohexene compared to 72 for cyclopentene and 100 for 1-hexene. In Brown's studies he noted isomerization on heating. To judge the scope of the isomerization he made use of cyclic alkenes. His experiments found that the boron was equilibrated on all of the available sites and tends to accumulate on the least hindered carbon. Brown developed a procedure to displace organic boranes to form cyclic alkenes proving to effectively convert exocyclic alkenes to endocyclic. An interesting example of this displacement procedure came with an adduct of 1-methylcyclohexene. By adding 1-hexene and diglyme to the dialkyl adduct the methylcyclohexyl group was displaced to give a product ratio of 77:23 1-methylcylohexene to 3-methylcyclohexene. Most relevant for our research Brown reported the product ratio for the hydroboration of t methylcyclohexene afforded 0.8% of the cis-2-cyclohexanol, 1.5% 1-methylcyclohexanol, and 97.7% of the trans-2-methylcyclohexanol preferred. The observation of the cis-2-methylcyclohexanol is interesting. It is indicative of either isomerization occurring, under Brown's reaction conditions, or the presence of impurities in the started alkene. We were interested in the effect of the cyclic alkene on the potential role of dynamic effects in hydroborations and sought to compare the energy surface for cyclic alkenes versus analogous acyclic alkenes. In this case we were able to compare the hydroboration of 1-methylcyclohexene with that of 2-methyl-2-butene. Later we will make a comparison with the hydroboration of 2-methylcyclohexene.

The most pertinent information for our research the findings reported for product ratio after the hydroboration of 0.3 mol of olefin with 0.125 mol of borane in diglyme. The outcome was analyzed to be 0.8 % of the *cis*-2-methylcyclohexanol, 1.5 % of 1-

methylcyclohexanol and 97.7 % of the preferred *trans*-2-methylcyclohexanol (Scheme **4.6**).

Scheme 4.6



Our current investigation was intended to contribute to the theoretical pathway in the reaction model of the hydroboration of 1-methylcyclohexene with BH_3 with an innovative prospective. Our hypothesis was to compare directly the barriers of a cyclic alkene and the acyclic analogous alkene, as well as, put side-by-side two different structural isomers of a cyclic alkene. In this case we were able to compare the hydroboration of 1-methylcyclohexene and 2-methyl-2-butene, and soon after we will make a comparison for the hydroboration of 3-methylcyclohexene.

A reaction coordinate diagram based on the calculated enthalpies and free energies is shown in Figure 4.3. We wanted to judge the experimental selectivity for the reaction against the predicted $\Delta\Delta G^{\ddagger}$ for transition states. To accomplish this, the hydroboration transition structures for the 1-methylcyclohexene reaction were located in the gas-phase G3B3, B3LYP/6-31G* and B3LYP/6-31+G** calculations. The approximate $\Delta\Delta G^{\ddagger}$ and $\Delta\Delta H^{\ddagger}$ of all the structures found by the three different methods are presented in Table 4.6. For our discussion we will refer to the G3B3 energies. Based

on their close match with other high level calculational methods like CCSD(T) with very large basis sets the hydroboration of propene with BH_3 (Chapter II).

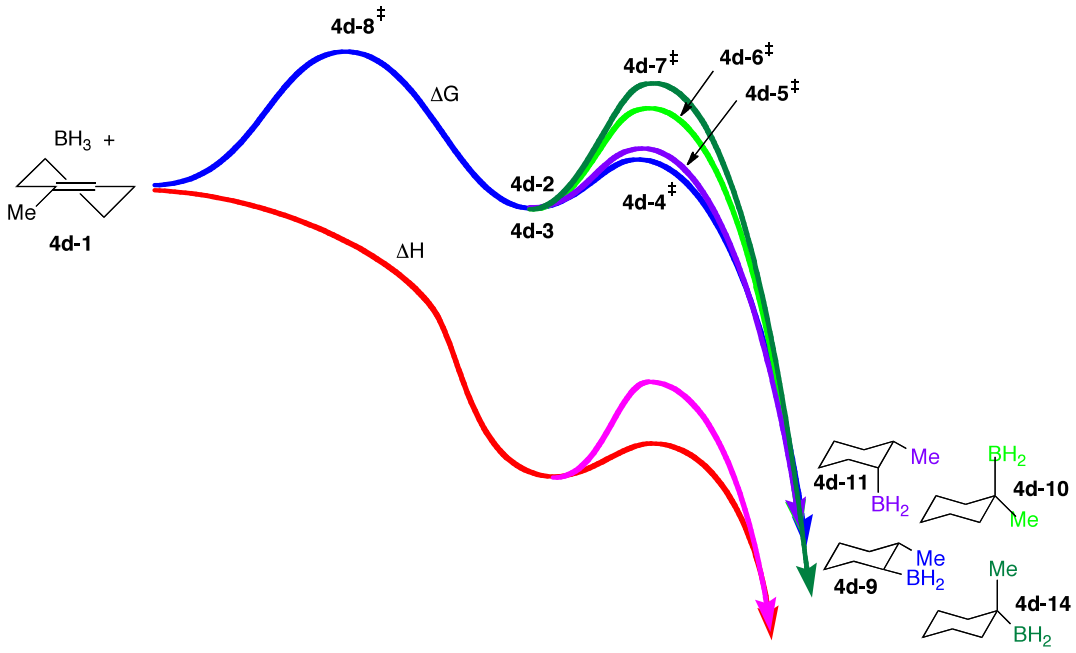


Figure 4.3. Reaction coordinate diagram for the hydroboration of 1-methylcyclohexene based on the predicted G3B3 enthalpies and free energies.

Two differences in energy had to be considered in this case to compare with experimental regioselectivity. Allowing for the shared like conformation of the 1-methycyclohexene there are two faces for the approach of the BH3 to the alkene it is necessary to consider the difference of energy anti-Markovnikov transition state and Markovnikov transition state for the BH_3 attack at each. The $\Delta\Delta G^{\ddagger}$ predicted for structure **4d-4**‡ and **4d-6**‡ is 2.6 kcal/mol and the $\Delta\Delta G^{\ddagger}$ predicted for structure **4d-5**‡ and **4d-7**‡ is 2.7 kcal/mol. The relative energetics for these structures are represented in Figure **4.3**. Preference for anti-Markovnikov can be consider in agreement with the

experimental percentage reported in the literature of (97.7 % and 0.8 %) 98.5 to 1.5 anti-Markovnikov to Markovnikov. Its notable that with both of the trisubstituted alkenes investigated the experimental product ratio matches up well with the theoretical calculations.. A difference between the two systems is that the π-complex **4d-2** or π-complex **4d-3** to the transition structure **4d-4**‡ is 3.7 kcal/mol with 1-methyl cyclohexene with the corresponding barrier in 2-methyl-2-butene was lower at 3.0 kcal/mol. The difference in the barriers can be expected to reflect the consequences of the afforded experimental selectivity. In fact 1-methylcyclohexene is slightly more selective than 2-methyl-2-butene when judging the anti-Markovnikov versus Markovnikov product. The difference in energy for the two possible anti-Markovnikov transition states is very small, 0.3 kcal/mol, when the difference in energy for the two possible facial attacks to form the Markovnikov transition states is 0.5 kcal/mol.

Table 4.6. Enthalpies and free energies for calculated structures for the hydroboration of BH_3 with 1-methylcyclohexene.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4d-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
4d-8‡	$\Delta G^{\ddagger} = 5.1$ $\Delta H^{\ddagger} = -3.5$	$\Delta G^{\ddagger} = 6.7$ $\Delta H^{\ddagger} = -2.2$	$\Delta G^{\ddagger} = 6.9$ $\Delta H^{\ddagger} = -1.5$
4d-2	$\Delta G = -1.8$ $\Delta H = -11.8$	$\Delta G = 3.3$ $\Delta H = -9.5$	$\Delta G = 4.8$ $\Delta H = -8.3$

Table 4.6. continued.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4d-3	ΔG = - 1.8 ΔH = - 11.8	ΔG = 3.3 ΔH = - 9.5	ΔG = 4.4 ΔH = - 8.3
4d-4‡	$\Delta G^{\ddagger}$ = 1.9 $\Delta H^{\ddagger}$ = - 10.1	$\Delta G^{\ddagger}$ = 8.0 $\Delta H^{\ddagger}$ = - 6.1	$\Delta G^{\ddagger}$ = 8.5 $\Delta H^{\ddagger}$ = - 5.6
4d-5‡	$\Delta G^{\ddagger}$ = 2.2 $\Delta H^{\ddagger}$ = - 7.5	$\Delta G^{\ddagger}$ = 8.1 $\Delta H^{\ddagger}$ = - 5.9	$\Delta G^{\ddagger}$ = 8.7 $\Delta H^{\ddagger}$ = - 5.4
4d-6‡	$\Delta G^{\ddagger}$ = 4.5 $\Delta H^{\ddagger}$ = - 7.5	$\Delta G^{\ddagger}$ = 10.3 $\Delta H^{\ddagger}$ = - 3.7	$\Delta G^{\ddagger}$ = 11.1 $\Delta H^{\ddagger}$ = - 3.0
4d-7‡	$\Delta G^{\ddagger}$ = 5.0 $\Delta H^{\ddagger}$ = - 7.0	$\Delta G^{\ddagger}$ = 10.6 $\Delta H^{\ddagger}$ = - 3.4	$\Delta G^{\ddagger}$ = 11.5 $\Delta H^{\ddagger}$ = - 2.6
4d-9	ΔG = - 15.4 ΔH = - 26.3	ΔG = -10.6 ΔH = - 25.2	ΔG = - 9.4 ΔH = - 24.1
4d-10	ΔG = -15.1 ΔH = - 26.2	ΔG = - 9.1 ΔH = - 23.8	ΔG = - 7.9 ΔH = - 22.6
4d-11	ΔG = - 14.8 ΔH = - 25.8	ΔG = - 9.5 ΔH = - 24.0	ΔG = - 8.4 ΔH = - 23.0
4d-12	ΔG = - 14.2 ΔH = - 25.2	ΔG = - 9.0 ΔH = - 23.4	ΔG = - 8.0 ΔH = - 22.4

Table 4.6 continued.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4d-13	ΔG = - 13.8 ΔH = - 25.0	ΔG = - 8.3 ΔH = - 23.0	ΔG = - 7.2 ΔH = - 21.9
4d-14	ΔG = - 13.1 ΔH = - 24.0	ΔG = - 7.3 ΔH = - 21.7	ΔG = - 6.1 ΔH = - 20.5

According to methods/basis set G3B3, B3LYP/6-31G* and B3LYP/6-31+G** calculations, they are relative to the starting material and expressed in kcal/mol. Energies are kcal/mol versus the separate starting materials

Table 4.7. Free energy for π-complexes at hydroboration transition states after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4d-2	ΔG = - 1.0	ΔG = 4.1	ΔG = 5.7
4d-3	ΔG = - 0.9	ΔG = 4.2	ΔG = 5.3
4d-4‡	$\Delta G^{‡}$ = 1.9	$\Delta G^{‡}$ = 8.0	$\Delta G^{‡}$ = 8.5
4d-5‡	$\Delta G^{‡}$ = 2.4	$\Delta G^{‡}$ = 8.3	$\Delta G^{‡}$ = 8.9
4d-6‡	$\Delta G^{‡}$ = 4.3	$\Delta G^{‡}$ = 10.1	$\Delta G^{‡}$ = 10.6
4d-7‡	$\Delta G^{‡}$ = 5.1	$\Delta G^{‡}$ = 10.8	$\Delta G^{‡}$ = 11.6

The predicted barriers discussed so far have not included any allowance for corrections of any. Explained previously, we found essential to fix the calculated energetics by allowing for the second-order perturbative anharmonic contributions to the vibrational energies and entropy since the magnitude of the $\Delta\Delta G^{\ddagger}$ is small side. For the π-complexes and product forming transition structures are shown in Table 4.7.

As a result of the anharmonic correction, the $\Delta\Delta G^{\ddagger}$ predicted for structure **4d-4**‡ versus **4d-6**‡ changed to 2.4 kcal/mol and the $\Delta\Delta G^{\ddagger}$ predicted for structure **4d-5**‡ and **4d-7**‡ stayed at 2.7 kcal/mol. The uncorrected versus the corrected $\Delta\Delta G^{\ddagger}$ for the competitive transition states can be found in Table **4.7**. Over the anharmonic corrections did not change the basic situation that the calculated and experimental selectivities are in reasonable agreement. This fits within the finding that transition state theory predicts the experimental selectivity in the hydroboration of 2-methyl-2-butene.

The $\Delta\Delta G^{\ddagger}$ predicted for the two anti-Markovnikov transition states, structures **4d-4**‡ and **4d-5**‡ when corrected is 0.5 kcal/mol. This value compares to the $\Delta\Delta G^{\ddagger}$ predicted for the two Markovnikov transition states, structure **4d-6**‡ and **4d-7**‡, which after the correction is 0.8 kcal/mol. The difference in the $\Delta\Delta G^{\ddagger}$ predicted after correcting for the perturbative anharmonic contributions is more consistent with the expected stability of the transition states according to the half chair attack preference. The difference in the energetics in the reaction of BH_3 with 1-methylcyclohexene after anharmonic correction can be observed by comparing the barriers in Figure 4.4.

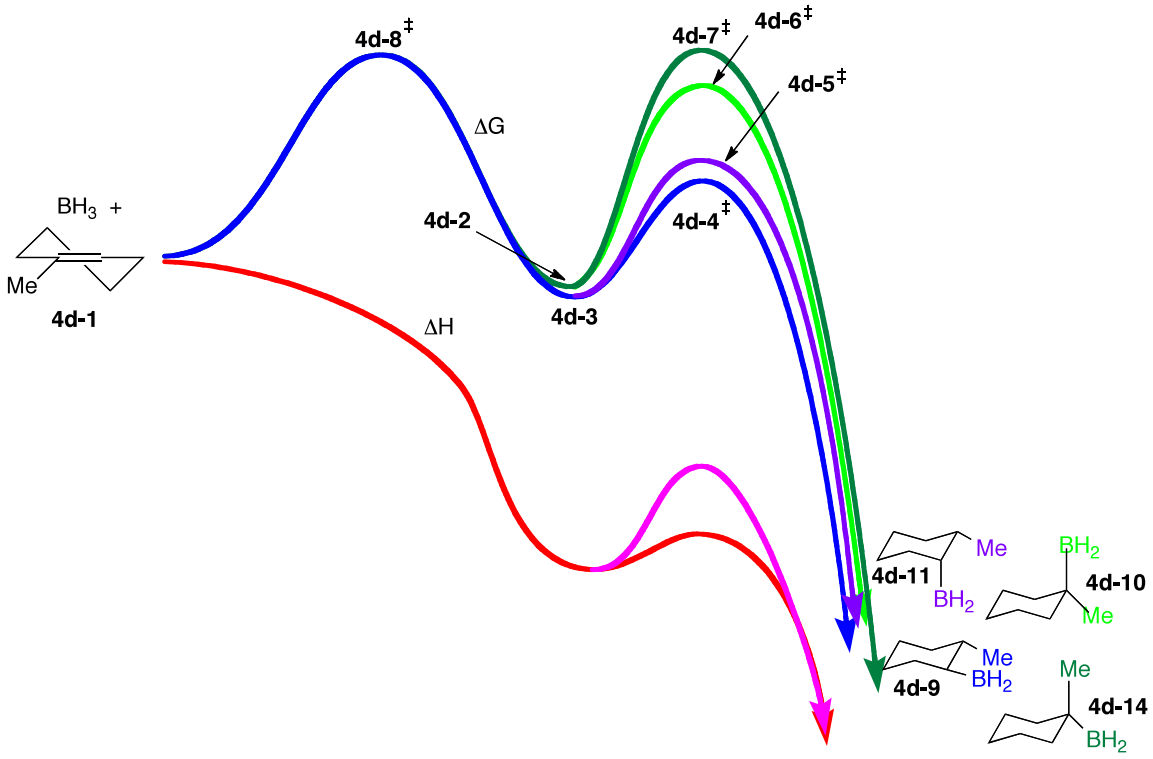


Figure 4.4. Calculated $\Delta\Delta G^{\ddagger}$ for transition states **4d-4**‡ versus **4d-6**‡, and, **4d-5**‡ versus **4d-7**‡ with and without the anharmonic contributions.

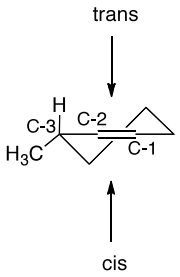
Overall, we find that the hydroboration of 1-methyl-cyclohexene is well predicted by transition state theory, as was the case in the hydroboration of 2-methyl-2-butene. A more apparent understanding of the consequences of including the perturbative anharmonic contributions when evaluating such little differences in energies was seen here.

Dynamics and Selectivity in the Hydroboration of 3-Methylcyclohexene with BH_3

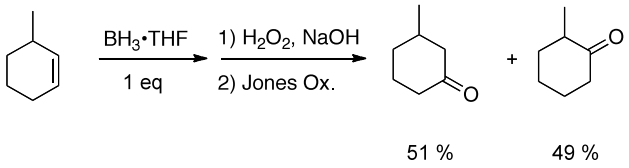
Calculated Pathway for the Hydroboratoin of 1-MethylcycolHexane with BH_3

The stereochemistry of hydroboration reactions with borane has been studied for several cyclic and bicyclic alkenes. Brown determined the directive effect of allylic substituents on cyclic alkenes. When 3-methyl-cycylohexene was hydroborated with

diborane in tetrahydrofuran, a mixture of 49% 2-methylcyclohexanone and 51% 3-methylcyclohexanone, was obtained after oxidative workup follow by a Jones procedure.[17b]

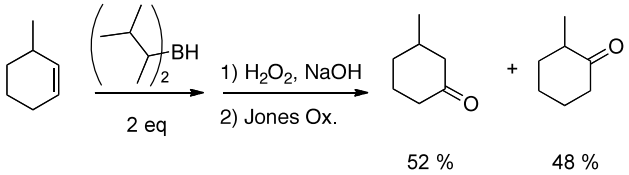


Scheme 4.7



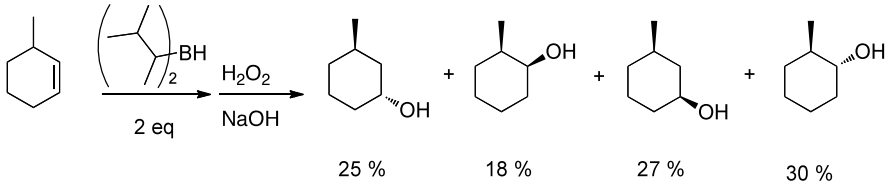
Brown found that selectivity increased little with a bulky hydroborating agent. When 3-methylcyclohexene was hydroborated with disiamylborane, after classic oxidation followed by further oxidation with a Jones procedure, the selectivity was 48% 2-methylcyclohexanone and 52% 3-methylcyclohexanone.

Scheme 4.8



Subsequently, Brown was able to resolve the oxidized blend of alcohols with a diglycerol capillary column. It was confirmed that when 3-methylcyclohexene is hydroborated with a bulky hydroborating agent, disiamylborane, 48% of the boron was added to C-2 and 52% was added to C-1. From the 48% addition, 18% formed the *cis*-2-methylcyclohexanol and 30% gave the *trans*-2-methylhexanol.

Scheme 4.9

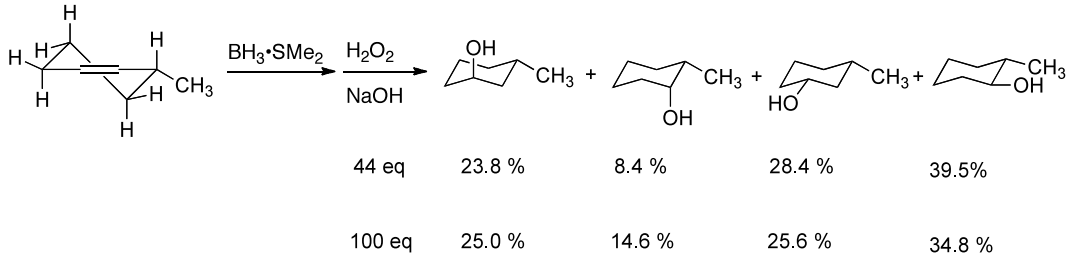


Brown generalized that the stereochemistry was not controlled by the stability of the product. The low experimental selectivity pointed by Brown for the hydroboration of 3-methylcyclohexene is striking and we explored this reaction further to establish if transition state theory fits with the experimental results. We sought to determine if is there a discrepancy between the experimental selectivity and transition state theory for this reaction. If so, do dynamic trajectories account for the observed selectivity?

Our initial goal was to establish the effect of excess borane on the product selectivity for the hydroboration of 3-methylcyclohexene. When this reaction done using 44 equivalents of borane•dimethylsulfide afforded, the product mixture after oxidation to the alcohol stage, was 47.9% of 2-methylcyclohexanol and 52.1% was 3-methylcyclohexanol. The 47.9% C-2 addition consisted of a combination of 8.4% of the *cis*-2-methylcyclohexanol and the 39.5% of the *trans*-2-methylhexanol. The rest of the

product was a combination of 28.4% of the boron addition to the C-1 position to be *cis*-3-methylcyclohexanol and 23.8% of *trans*-3-methylcyclohexanol. The 52.1% of the C-3 addition consisted of a combination of 28.4% of cis-3-methylcyclohexanol and 20.83% of trans-3-methylcyclohexanol. When the reaction was performed with a larger excess of borane•dimethylsulfide, 100 equivalence we obtained a combination of 49.4% of 2-methylcyclohexanol and 50.6% 3-methylcyclohexanol. The 49.4% C-2 addition consisted of a combination of 14.6% the *cis*-2-methylcyclohexanol and 34.8% *trans*-2-methylhexanol. The 50.6% corresponding to boron addition at the C-1 position was found to be a combination of 25.6% *cis*-3-methylcyclohexanol and 25.0% *trans*-3-methylcyclohexanol.

Scheme 4.10



Borane•dimethylsulfide was the hydroborating agent selected for the research completed for 3-methylcyclohexene after taking into consideration the experimental advantages seen over other possibilities in the hydroboration of BH_3/2-methyl-2-butene. Smaller alkenes the hydroboration of methylcyclohexene has the advantage that lost of the product alcohol of the aqueous layer after oxidation is expected to be insignificant. This hydroboration could be performed using neat borane which allowed for direct

analysis of the reaction by ^{1}H NMR of and an oxidized aliquot extracted with toluene d_8 ^{1}H NMR signals observed for the carbonyl protons of the product's *cis*-2-methylcyclohexanol and *trans*-2-methylhexanol was identified based on known spectra. A spectrum of a mixture of *cis*-3-methylcyclohexanol and *trans*-3-methylhexanol was also available. The ^{1}H NMR peaks corresponding to the carbonyl protons of that spectra were compared to the findings of previous research on the conformational equilibria of trans-3-X-cyclohexanols,[ref] which provided detail NMR of *trans*-3-methylhexanol leading to the final identification.

Obtaining an accurate experimental selectivity for the hydroboration of 3-methylcyclochexene was not as straight forward as had been anticipated. As in the hydroboration of 2-methyl-2-butene we observe by ^{1}H NMR that the reaction mixture was not a clean combination of the anticipated alcohols. Some of the impurities appeared to isomerization of the alkyl or dialkyl borane. This was concluded after analyzing the known ^{1}H NMR some of the possible product isomers. All of the percentages of the products change significantly after a week as shown below. For a hydroboration of 3-methylcyclohexene with 100 equivalents of borane, that was left for over a week, the products ratio changed from 25.0% *trans*-3-methylcyclohexanol at short reaction times to 14.7% in the neat reaction, from 14.6% the *cis*-2-methylcyclohexanol when the reaction is pure to 6.3%, from 25.6% *cis*-3-methylcyclohexanol to 17.2%, and 34.8% *trans*-2-methylhexanol to 20.8%. The reaction in plain 100 equivalents of borane changed from a nearly equal mixture 2-methylcyclohexanol and 3-methylcyclohexanol at a short reaction time to a mixture of

27.1% 2-methylcyclohexanol, 31.9% 3-methylcyclohexanol, along with 41% of other alcohol and the reaction continued for over a week.

Another example isomerization was observed for the hydroboration of 3-methylcyclohexene with 0.3 equivalent of borane, and the reaction was left for over a two day period. The products ratio obtained was 12.2% *trans*-3-methylcyclohexanol, 3.1% *cis*-2-methylcyclohexanol, 26.0% *cis*-3-methylcyclohexanol (the integration to estimate this percentage combined the desired peak plus other impurities that could not be avoided), and 5.0% *trans*-2-methylhexanol. Therefore, in a 0.2 equivalents of borane reaction gives 49% of 2-methylcyclohexanol, but if the reaction mixture is left for a long period of time at 22 °C with excess alkene the mixture changes to 7.8% 2-methylcyclohexanol and a lot more impurities are observed (some identified as isomers). It is particular noticeable that the 2-methycyclohexanol dropped drastically in amount. It was observed that isomerization was unavoidable when an excess of alkene is added. For this reason, the reaction mixture could not be determined accurately when using small amounts of borane.

With experimental results in hand, we turned to evaluating the ability of transition state theory to predict the selectivity in this reaction. To determine the predictions of transition state theory a series of structures was located in gas phase calculations for integration of 3-methylcyclohexene with BH_3, using B3LYP/6-31G*, B3LYP/6-31+G** and B3LYP/CBSB7 (Figure **4.8**). Single point energies with a variety of method/basis set were then obtained for each of these structures using the geometries obtained from B3LYP/6-31+G**. The methods/basis sets used for the single

point calculations of structures located for all transition sates, starting material and complexes were: CCSD(T)/6-311+G**, CCSD(T)/6-31+G**, CCSD(T)/aug-cc-pvdz, CCSD(T)/cc-pvdz, MO5/631+G**, MP4(sdq)/aug-cc-pvdz, MP4(sdtq)/cc-pvtz, B1B95/6-31+G**, MPWLYP/6-31+G**, MPWPW91/6-31+G**, TPSSTPSS/cc-pvtz, MO5/631+G**. In the case of G3B3 energy calculations, the geometries were calculated using B3LYP/6-31G*. The methods/basis sets used were chosen based on the margin of RMS error predicted for the previously discussed energy calculations for the hydroboration of propene with BH_3. A summary of all the predicted enthalpies and free energies with the variety of gas-phase computational approaches is organized in the tables below and contains the values with methyl group in axial position relative to the methyl group in equatorial position, and it includes the free energy after anharmonic adjustment, which we will discuss later; Table **4.9** combines the energies for structures located for all complexes formed from BH_3/3-methylcyclohexene; finally, Tables **4.10** and **4.11** contain transition structures located with the methyl group with the equatorial and axial positions, respectively.

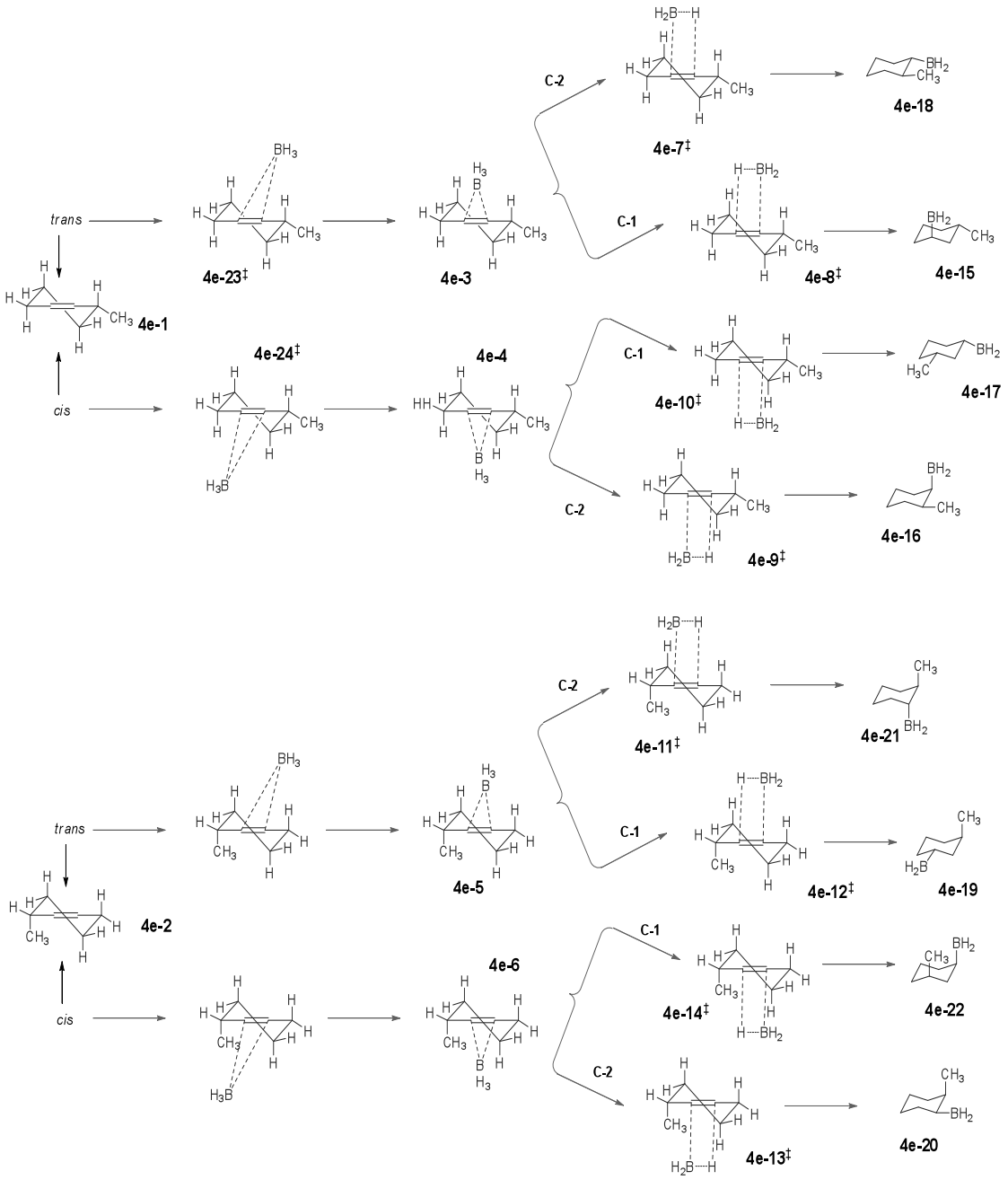


Figure 4.5. Key for the structures calculated for system 3-methylcyclohexene/BH_3

More limited set of methods and basis sets employed to study the product structures. These included G3B3, B3LYP/6-31G*, B3LYP/6-31+G**, CBS-QB3, CCSD(T)/6-311+G**, CCSD(T)/aug-cc-pvdz, MP4(sdq)/aug-cc-pvdz, MP4(sdtq)/cc-pvtz,. The more limited sets of calculations was because the stabilities of the products were of lower importance for the purpose of the study. A summary of all the predicted enthalpies and free energies is organized in all the tables with a variety of gas-phase computational approaches expressed in kcal/mol can be found in Tables **4.11,4.12, and 4.13** contains the structures located for the products with the methyl in the equatorial position and axial position, respectively. To better understand these tables the reader should refer to diagram **1**.

Subsequent to determining the barriers from complexes for the formation of all potential products in the hydroboration of 3-methylcyclohexene, we want to explore in detail other possibilities to explain the experimental selectivity. So far the kinetic selectivity in hydroboration is view as the result of the two differing transition state barriers that lead to the alternative reaction products. This does not consider the fact that an exothermic association process and an entropic barrier might be involved. This was applied to this case without considering the fact that an exothermic association process with an entropic barrier might be involved.

Table 4.8. Calculated enthalpies and free energy values for 3-methylcyclohexene with methyl in axial position relative to the methyl in equatorial position.

Structure / Method / Basis Set	**4e-1**	**4e-2**	**4e-2** corrected
G3B3	ΔG = 0.0 ΔH = 0.0	ΔG = 0.6 ΔH = 0.6	ΔG = 0.9
B3LYP/6-31G*	ΔG = 0.0 ΔH = 0.0	ΔG = 0.8 ΔH = 0.7	ΔG = 1.1
B3LYP/6-31+G**	ΔG = 0.0 ΔH = 0.0	ΔG = 0.9 ΔH = 0.8	ΔG = 1.2
CBS-QB3	ΔG = 0.0 ΔH = 0.0	ΔG = 0.6 ΔH = 0.6	ΔG = 0.9
CCSD(T)/6-311+G**	ΔG = 0.0 ΔH = 0.0	ΔG = 0.7 ΔH = 0.7	ΔG = 1.0
CCSD(T/)6-31+G**	ΔG = 0.0 ΔH = 0.0	ΔG = 0.8 ΔH = 0.8	ΔG = 1.1
CCSD(T)/aug-cc-pvdz	ΔG = 0.0 ΔH = 0.0	ΔG = 0.7 ΔH = 0.7	ΔG = 1.0
CCSD(T)/cc-pvdz	ΔG = 0.0 ΔH = 0.0	ΔG = 0.7 ΔH = 0.7	ΔG = 1.0

Table 4.8 continued.

Structure / Method / Basis Set	**4e-1**	**4e-2**	**4e-2** corrected
MO5/631+G**	ΔG = 0.0 ΔH = 0.0	ΔG = 0.9 ΔH = 0.9	ΔG = 1.2
MP4(sdq)/aug-cc-pvdz	ΔG = 0.0 ΔH = 0.0	ΔG = 0.7 ΔH = 0.7	ΔG =1.0
MP4(sdtq)/cc-pvtz	ΔG = 0.0 ΔH = 0.0	ΔG = 26.4 ΔH = 26.4	ΔG = 26.7
B1B95/6-31+G**	ΔG = 0.0 ΔH = 0.0	ΔG = 0.8 ΔH = 0.8	ΔG = 1.1
MPWLYP/6-31+G**	ΔG = 0.0 ΔH = 0.0	ΔG = 0.9 ΔH = 0.9	ΔG = 1.2
MPWPW91/6-31+G**	ΔG = 0.0 ΔH = 0.0	ΔG = 0.8 ΔH = 0.8	ΔG = 1.1
TPSSTPSS/cc-pvtz	ΔG = 0.0 ΔH = 0.0	ΔG = 45.0 ΔH = 45.0	ΔG = 45.3

Table 4.9. Calculated enthalpies and free energies for all structures located for the complexes formed from combining BH_3 with 3-methylcyclohexene.

Structure / Method / Basis Set	**4e-3**	**4e-4**	**4e-5**	**4e-6**
G3B3	ΔG = - 0.9 ΔH = - 11.1	ΔG = - 0.4 ΔH = - 10.4	ΔG = - 0.1 ΔH = - 10.2	ΔG = 1.2 ΔH = - 9.3
B3LYP/6-31G*	ΔG = 2.8 ΔH = - 10.1	ΔG = 3.2 ΔH = - 9.5	ΔG = 3.7 ΔH = - 9.1	ΔG = 5.2 ΔH = - 8.2
B3LYP/6-31+G**	ΔG = 4.3 ΔH = - 8.6	ΔG = 4.7 ΔH = - 7.8	ΔG = 5.4 ΔH = - 7.5	ΔG = 6.9 ΔH = - 6.5
CBS-QB3	ΔG = - 0.6 ΔH = - 10.8	ΔG = 1.5 ΔH = - 9.0	ΔG = - 0.2 ΔH = - 10.1	ΔG = 1.5 ΔH = - 9.0
CCSD(T)/6-311+G**	ΔG = 3.3 ΔH = - 7.0	ΔG = 1.1 ΔH = - 8.9	ΔG = 0.3 ΔH = - 9.8	ΔG = 1.8 ΔH = - 8.9
CCSD(T/)6-31+G**	ΔG = 2.5 ΔH = - 7.8	ΔG = 3.0 ΔH = - 7.0	ΔG = 3.4 ΔH = - 6.8	ΔG = 5.1 ΔH = - 5.6
CCSD(T)/aug-cc-pvdz	ΔG = 2.9 ΔH = - 7.4	ΔG = 0.6 ΔH = - 9.3	ΔG = - 0.3 ΔH = - 10.5	ΔG = 1.1 ΔH = - 9.6
CCSD(T)/cc-pvdz	ΔG = 1.1 ΔH = - 9.2	ΔG = 1.6 ΔH = - 8.4	ΔG = 1.1 ΔH = - 9.0	ΔG = 3.5 ΔH = - 7.2

Table 4.9. continued.

Structure / Method / Basis Set	**4e-3**	**4e-4**	**4e-5**	**4e-6**
MO5/631+G**	ΔG = 1.7 ΔH = - 8.5	ΔG = 1.7 ΔH = - 8.3	ΔG = 3.0 ΔH = - 7.2	ΔG = 3.7 ΔH = - 129.1
MP4(sdq)/aug-cc-pvdz	ΔG = 7.6 ΔH = - 2.7	ΔG = 8.0 ΔH = - 1.9	ΔG = 8.5 ΔH = - 1.7	ΔG = 9.9 ΔH = - 0.8
MP4(sdtq)/cc-pvtz	ΔG = 0.5 ΔH = - 9.8	ΔG = 0.9 ΔH = - 9.1	ΔG = 1.4 ΔH = - 8.8	ΔG = 2.8 ΔH = - 7.9
B1B95/6-31+G**	ΔG = - 1.8 ΔH = - 12.1	ΔG = - 1.9 ΔH = - 11.9	ΔG = - 0.8 ΔH = - 10.9	ΔG = - 0.1 ΔH = - 10.8
MPWLYP/6-31+G**	ΔG = 2.9 ΔH = - 7.4	ΔG = 3.3 ΔH = - 6.7	ΔG = 4.0 ΔH = - 6.2	ΔG = 5.4 ΔH = - 5.2
MPWPW91/6-31+G**	ΔG = - 1.1 ΔH = - 11.4	ΔG = - 1.0 ΔH = - 11.0	ΔG = - 0.1 ΔH = - 10.2	ΔG = 1.0 ΔH = - 9.6
TPSSTPSS/cc-pvtz	ΔG = 43.2 ΔH = 33.0	ΔG = 43.6 ΔH = 34.6	ΔG = 44.4 ΔH = 34.2	ΔG = 45.6 ΔH = 34.9

Table 4.10. Calculated enthalpies and free energies for transition state structures located for the reaction of BH_3 with 3-methylcyclohexene with the methyl in the equatorial position.

Method / Basis Set \ Structure	**4e-7**	**4e-8**	**4e-9**	**4e-10**
G3B3	$\Delta G^{\ddagger}$ = 2.7 $\Delta H^{\ddagger}$ = - 9.0	$\Delta G^{\ddagger}$ = 2.7 $\Delta H^{\ddagger}$ = - 8.9	$\Delta G^{\ddagger}$ = 2.3 $\Delta H^{\ddagger}$ = - 9.2	$\Delta G^{\ddagger}$ = 2.3 $\Delta H^{\ddagger}$ = - 9.0
B3LYP/6-31G*	$\Delta G^{\ddagger}$ = 6.9 $\Delta H^{\ddagger}$ = - 6.9	$\Delta G^{\ddagger}$ = 6.9 $\Delta H^{\ddagger}$ = - 6.9	$\Delta G^{\ddagger}$ = 6.9 $\Delta H^{\ddagger}$ = - 6.9	$\Delta G^{\ddagger}$ = 6.9 $\Delta H^{\ddagger}$ = - 7.0
B3LYP/6-31+G**	$\Delta G^{\ddagger}$ = 7.9 $\Delta H^{\ddagger}$ = - 5.8	$\Delta G^{\ddagger}$ = 7.9 $\Delta H^{\ddagger}$ = - 5.8	$\Delta G^{\ddagger}$ = 8.1 $\Delta H^{\ddagger}$ = - 5.7	$\Delta G^{\ddagger}$ = 8.1 $\Delta H^{\ddagger}$ = - 5.8
CBS-QB3	$\Delta G^{\ddagger}$ = 3.1 $\Delta H^{\ddagger}$ = - 8.6	$\Delta G^{\ddagger}$ = 3.1 $\Delta H^{\ddagger}$ = - 8.6	$\Delta G^{\ddagger}$ = 2.9 $\Delta H^{\ddagger}$ = - 8.8	$\Delta G^{\ddagger}$ = 3.1 $\Delta H^{\ddagger}$ = - 8.7
CCSD(T)/6-311+G**	$\Delta G^{\ddagger}$ = 3.2 $\Delta H^{\ddagger}$ = - 8.5	$\Delta G^{\ddagger}$ = 3.1 $\Delta H^{\ddagger}$ = - 8.5	$\Delta G^{\ddagger}$ = 3.1 $\Delta H^{\ddagger}$ = - 8.7	$\Delta G^{\ddagger}$ = 3.4 $\Delta H^{\ddagger}$ = - 8.5
CCSD(T)/6-31+G**	$\Delta G^{\ddagger}$ = 6.3 $\Delta H^{\ddagger}$ = - 5.4	$\Delta G^{\ddagger}$ = 6.2 $\Delta H^{\ddagger}$ = - 5.5	$\Delta G^{\ddagger}$ = 6.2 $\Delta H^{\ddagger}$ = - 5.6	$\Delta G^{\ddagger}$ = 6.5 $\Delta H^{\ddagger}$ = - 5.3
CCSD(T)/aug-cc-pvdz	$\Delta G^{\ddagger}$ = 3.3 $\Delta H^{\ddagger}$ = - 8.4	$\Delta G^{\ddagger}$ = 3.3 $\Delta H^{\ddagger}$ = - 8.4	$\Delta G^{\ddagger}$ = 3.3 $\Delta H^{\ddagger}$ = - 8.6	$\Delta G^{\ddagger}$ = 3.3 $\Delta H^{\ddagger}$ = - 8.6
CCSD(T)/cc-pvdz	ΔG = 5.0 ΔH = - 6.7	ΔG = 5.0 ΔH = - 6.7	ΔG = 5.0 ΔH = - 6.8	ΔG = 5.1 ΔH = - 6.7

Table 4.10 continued.

Structure / Method / Basis Set	**4e-7**	**4e-8**	**4e-9**	**4e-10**
MO5/631+G**	$\Delta G^{\ddagger}$ = 0.4 $\Delta H^{\ddagger}$ = - 11.3	$\Delta G^{\ddagger}$ = 0.3 $\Delta H^{\ddagger}$ = - 11.4	$\Delta G^{\ddagger}$ = 0.3 $\Delta H^{\ddagger}$ = - 11.4	$\Delta G^{\ddagger}$ = 0.6 $\Delta H^{\ddagger}$ = - 11.3
MP4(sdq)/aug-cc-pvdz	$\Delta G^{\ddagger}$ = 5.3 $\Delta H^{\ddagger}$ = - 6.4	$\Delta G^{\ddagger}$ = 5.3 $\Delta H^{\ddagger}$ = - 6.4	$\Delta G^{\ddagger}$ = 5.3 $\Delta H^{\ddagger}$ = - 6.5	$\Delta G^{\ddagger}$ = 5.3 $\Delta H^{\ddagger}$ = - 6.5
MP4(sdtq)/cc-pvtz	$\Delta G^{\ddagger}$ = 4.0 $\Delta H^{\ddagger}$ = -7.7	$\Delta G^{\ddagger}$ = 4.4 $\Delta H^{\ddagger}$ = - 7.7	$\Delta G^{\ddagger}$ = 3.9 $\Delta H^{\ddagger}$ = 17.9	$\Delta G^{\ddagger}$ = 4.1 $\Delta H^{\ddagger}$ = - 7.8
B1B95/6-31+G**	$\Delta G^{\ddagger}$ = - 1.3 $\Delta H^{\ddagger}$ = - 13.0	$\Delta G^{\ddagger}$ = - 1.4 $\Delta H^{\ddagger}$ = - 13.0	$\Delta G^{\ddagger}$ = - 1.4 $\Delta H^{\ddagger}$ = - 13.2	$\Delta G^{\ddagger}$ = - 1.4 $\Delta H^{\ddagger}$ = - 13.2
MPWLYP/6-31+G**	$\Delta G^{\ddagger}$ = 6.4 $\Delta H^{\ddagger}$ = - 5.3	$\Delta G^{\ddagger}$ = 6.5 $\Delta H^{\ddagger}$ = - 5.2	$\Delta G^{\ddagger}$ = 3.5 $\Delta H^{\ddagger}$ = - 8.3	$\Delta G^{\ddagger}$ = 6.6 $\Delta H^{\ddagger}$ = - 5.3
MPWPW91/6-31+G**	$\Delta G^{\ddagger}$ = - 0.1 $\Delta H^{\ddagger}$ = - 11.8	$\Delta G^{\ddagger}$ = - 0.2 $\Delta H^{\ddagger}$ = - 11.9	$\Delta G^{\ddagger}$ = - 0.1 $\Delta H^{\ddagger}$ = - 11.9	$\Delta G^{\ddagger}$ = - 0.01 $\Delta H^{\ddagger}$ = - 11.9
TPSSTPSS/cc-pvtz	$\Delta G^{\ddagger}$ = 46.5 $\Delta H^{\ddagger}$ = 34.8	$\Delta G^{\ddagger}$ = 46.4 $\Delta H^{\ddagger}$ = 34.7	$\Delta G^{\ddagger}$ = 46.5 $\Delta H^{\ddagger}$ = 34.7	$\Delta G^{\ddagger}$ = 46.6 $\Delta H^{\ddagger}$ = 34.8

Table 4.11. Calculated enthalpies and free energies for transition structures located for the products of the reaction of BH_3 with 3-methylcyclohexene with the methyl in the axial position.

Structure / Method / Basis Set	**4e-11**	**4e-12**	**4e-13**	**4e-14**
G3B3	$\Delta G^{\ddagger}$ = 3.7 $\Delta H^{\ddagger}$ = - 8.0	$\Delta G^{\ddagger}$ = 4.2 $\Delta H^{\ddagger}$ = - 7.6	$\Delta G^{\ddagger}$ = 2.6 $\Delta H^{\ddagger}$ = - 9.2	$\Delta G^{\ddagger}$ = 2.8 $\Delta H^{\ddagger}$ = - 9.0
B3LYP/6-31G*	$\Delta G^{\ddagger}$ = 8.2 $\Delta H^{\ddagger}$ = - 5.7	$\Delta G^{\ddagger}$ = 8.5 $\Delta H^{\ddagger}$ = - 5.4	$\Delta G^{\ddagger}$ = 8.8 $\Delta H^{\ddagger}$ = - 5.1	$\Delta G^{\ddagger}$ = 8.7 $\Delta H^{\ddagger}$ = - 5.2
B3LYP/6-31+G**	$\Delta G^{\ddagger}$ = 9.3 $\Delta H^{\ddagger}$ = - 4.5	$\Delta G^{\ddagger}$ = 9.7 $\Delta H^{\ddagger}$ = - 4.2	$\Delta G^{\ddagger}$ = 10.0 $\Delta H^{\ddagger}$ = - 3.8	$\Delta G^{\ddagger}$ = 10.0 $\Delta H^{\ddagger}$ = - 4.0
CBS-QB3	$\Delta G^{\ddagger}$ = 4.0 $\Delta H^{\ddagger}$ = - 7.7	$\Delta G^{\ddagger}$ = 4.5 $\Delta H^{\ddagger}$ = - 7.2	$\Delta G^{\ddagger}$ = 4.6 $\Delta H^{\ddagger}$ = - 7.1	$\Delta G^{\ddagger}$ = 4.5 $\Delta H^{\ddagger}$ = - 7.3
CCSD(T)/6-311+G**	$\Delta G^{\ddagger}$ = 4.2 $\Delta H^{\ddagger}$ = - 7.5	$\Delta G^{\ddagger}$ = 4.7 $\Delta H^{\ddagger}$ = - 7.0	$\Delta G^{\ddagger}$ = 4.9 $\Delta H^{\ddagger}$ = - 6.8	$\Delta G^{\ddagger}$ = 4.9 $\Delta H^{\ddagger}$ = - 7.0
CCSD(T)/6-31+G**	$\Delta G^{\ddagger}$ = 7.8 $\Delta H^{\ddagger}$ = - 3.9	$\Delta G^{\ddagger}$ = 7.9 $\Delta H^{\ddagger}$ = - 3.8	$\Delta G^{\ddagger}$ = 8.2 $\Delta H^{\ddagger}$ = - 3.5	$\Delta G^{\ddagger}$ = 8.1 $\Delta H^{\ddagger}$ = - 3.7
CCSD(T)/aug-cc-pvdz	$\Delta G^{\ddagger}$ = 4.4 $\Delta H^{\ddagger}$ = - 7.4	$\Delta G^{\ddagger}$ = 4.7 $\Delta H^{\ddagger}$ = - 6.9	$\Delta G^{\ddagger}$ = 4.8 $\Delta H^{\ddagger}$ = - 6.9	$\Delta G^{\ddagger}$ = 4.7 $\Delta H^{\ddagger}$ = - 7.2
CCSD(T)/cc-pvdz	$\Delta G^{\ddagger}$ = 6.1 $\Delta H^{\ddagger}$ = - 5.6	$\Delta G^{\ddagger}$ = 6.5 $\Delta H^{\ddagger}$ = - 5.1	$\Delta G^{\ddagger}$ = 6.7 $\Delta H^{\ddagger}$ = - 5.0	$\Delta G^{\ddagger}$ = 6.6 $\Delta H^{\ddagger}$ = - 5.2

Table 4.11 continued.

Structure / Method / Basis Set	**4e-11**	**4e-12**	**4e-13**	**4e-14**
MO5/631+G**	$\Delta G^{\ddagger}$= 1.6 $\Delta H^{\ddagger}$= - 10.2	$\Delta G^{\ddagger}$= 2.0 $\Delta H^{\ddagger}$= - 9.7	$\Delta G^{\ddagger}$= 2.3 $\Delta H^{\ddagger}$= - 9.4	$\Delta G^{\ddagger}$= 2.3 $\Delta H^{\ddagger}$= - 9.5
MP4(sdq)/aug-cc-pvdz	$\Delta G^{\ddagger}$= 6.4 $\Delta H^{\ddagger}$= - 5.3	$\Delta G^{\ddagger}$= 6.8 $\Delta H^{\ddagger}$= - 4.9	$\Delta G^{\ddagger}$= 6.9 $\Delta H^{\ddagger}$= - 4.8	$\Delta G^{\ddagger}$= 6.8 $\Delta H^{\ddagger}$= - 4.9
MP4(sdtq)/cc-pvtz	$\Delta G^{\ddagger}$= 5.1 $\Delta H^{\ddagger}$= - 6.7	$\Delta G^{\ddagger}$= 5.5 $\Delta H^{\ddagger}$= - 6.2	$\Delta G^{\ddagger}$= 5.7 $\Delta H^{\ddagger}$= - 6.0	$\Delta G^{\ddagger}$= 5.6 $\Delta H^{\ddagger}$= - 6.3
B1B95/6-31+G**	$\Delta G^{\ddagger}$= - 0.2 $\Delta H^{\ddagger}$= - 12.0	$\Delta G^{\ddagger}$= 0.2 $\Delta H^{\ddagger}$= - 11.5	$\Delta G^{\ddagger}$= 0.4 $\Delta H^{\ddagger}$= - 11.4	$\Delta G^{\ddagger}$= 0.5 $\Delta H^{\ddagger}$= - 11.4
MPWLYP/6-31+G**	$\Delta G^{\ddagger}$= 7.8 $\Delta H^{\ddagger}$= - 4.0	$\Delta G^{\ddagger}$= 8.2 $\Delta H^{\ddagger}$= - 3.5	$\Delta G^{\ddagger}$= 8.4 $\Delta H^{\ddagger}$= - 3.3	$\Delta G^{\ddagger}$= 8.4 $\Delta H^{\ddagger}$= - 3.4
MPWPW91/6-31+G**	$\Delta G^{\ddagger}$= 1.0 $\Delta H^{\ddagger}$= - 10.8	$\Delta G^{\ddagger}$= 1.4 $\Delta H^{\ddagger}$= - 10.3	$\Delta G^{\ddagger}$= 1.8 $\Delta H^{\ddagger}$= - 9.9	$\Delta G^{\ddagger}$= 1.6 $\Delta H^{\ddagger}$= - 10.3
TPSSTPSS/cc-pvtz	$\Delta G^{\ddagger}$= 47.5 $\Delta H^{\ddagger}$= 35.7	$\Delta G^{\ddagger}$= 48.0 $\Delta H^{\ddagger}$= 36.3	$\Delta G^{\ddagger}$= 48.1 $\Delta H^{\ddagger}$= 36.4	$\Delta G^{\ddagger}$= 48.0 $\Delta H^{\ddagger}$= 36.1

Table 4.12. Calculated enthalpies and free energies for product structures located for the reaction of BH_3 with 3-methylcyclohexene with the methyl in the equatorial position.

Structure / Method / Basis Set	**4e-15**	**4e-16**	**4e-17**	**4e-18**
G3B3	ΔG = - 17.8 ΔH = - 28.6	ΔG = - 16.8 ΔH = - 27.6	ΔG = - 17.8 ΔH = - 28.6	ΔG = - 17.4 ΔH = - 28.1
B3LYP/6-31G*	ΔG = - 14.2 ΔH = - 28.4	ΔG = - 12.8 ΔH = - 27.1	ΔG = - 14.3 ΔH = - 28.5	ΔG = - 14.0 ΔH = - 28.4
B3LYP/6-31+G**	ΔG = - 12.7 ΔH = - 26.9	ΔG = - 11.2 ΔH = - 25.5	ΔG = - 12.8 ΔH = - 26.8	ΔG = - 12.2 ΔH = - 26.6
CBS-QB3	ΔG = - 17.4 ΔH = - 28.4	ΔG = - 16.4 ΔH = - 27.4	ΔG = - 17.3 ΔH = - 27.8	ΔG = - 17.2 ΔH = - 28.0
CCSD(T)/6-311+G**	ΔG = - 18.2 ΔH = - 29.1	ΔG = - 17.0 ΔH = - 28.0	ΔG = - 18.0 ΔH = - 28.5	ΔG = - 18.0 ΔH = - 28.8
CCSD(T)/aug-cc-pvdz	ΔG = - 18.9 ΔH = - 29.8	ΔG = - 17.9 ΔH = - 28.9	ΔG = - 18.6 ΔH = - 29.1	ΔG = - 18.5 ΔH = - 29.3
MP4(sdq)/aug-cc-pvdz	ΔG = - 19.1 ΔH = - 30.0	ΔG = - 18.0 ΔH = - 29.0	ΔG = - 18.8 ΔH = - 29.3	ΔG = - 18.6 ΔH = - 29.4
MP4(sdtq)/cc-pvtz	ΔG = - 17.9 ΔH = - 28.8	ΔG = - 16.7 ΔH = - 27.7	ΔG = - 17.6 ΔH = - 28.1	ΔG = - 17.4 ΔH = - 28.2

Table 4.13. Calculated enthalpies and free energies for structures located for the products of the reaction of BH_3 with 3-methylcyclohexene with the methyl in the axial position.

Structure / Method / Basis Set	**4e-19**	**4e-20**	**4e-21**	**4e-22**
G3B3	ΔG = - 15.5 ΔH = - 26.2	ΔG = - 16.2 ΔH = - 27.0	ΔG = - 16.6 ΔH = - 27.8	ΔG = - 15.8 ΔH = - 26.8
B3LYP/6-31G*	ΔG = - 11.8 ΔH = - 26.4	ΔG = - 12.3 ΔH = - 26.5	ΔG = - 11.8 ΔH = - 26.5	ΔG = - 11.6 ΔH = - 26.1
B3LYP/6-31+G**	ΔG = - 10.3 ΔH = - 24.6	ΔG = - 10.7 ΔH = - 24.9	ΔG = - 10.3 ΔH = - 24.8	ΔG = - 10.0 ΔH = - 24.5
CBS-QB3	ΔG = - 15.4 ΔH = - 26.0	ΔG = - 15.9 ΔH = - 26.8	ΔG = - 16.3 ΔH = - 27.3	ΔG = - 15.4 ΔH = - 26.5
CCSD(T)/6-311+G**	ΔG = - 16.1 ΔH = - 26.7	ΔG = - 16.6 ΔH = - 27.6	ΔG = - 17.0 ΔH = - 28.0	ΔG = - 16.1 ΔH = - 27.2
CCSD(T)/aug-cc-pvdz	ΔG = - 16.6 ΔH = - 27.2	ΔG = - 17.2 ΔH = - 28.1	ΔG = - 17.9 ΔH = - 28.9	ΔG = - 16.8 ΔH = - 27.9
MP4(sdq)/aug-cc-pvdz	ΔG = - 16.7 ΔH = - 300.7	ΔG = - 17.3 ΔH = - 28.3	ΔG = - 17.9 ΔH = - 29.0	ΔG = - 17.0 ΔH = - 28.0
MP4(sdtq)/cc-pvtz	ΔG = - 15.6 ΔH = - 26.2	ΔG = - 16.2 ΔH = - 30.2	ΔG = - 19.0 ΔH = - 27.8	ΔG = - 15.8 ΔH = - 26.9

As previously found with other alkenes, there is no enthalpic barrier for formation of any of the olefin – BH_3 π-complexes (**4e-3** to **4e-6**) from separate 3-methylcyclohexene and BH_3 molecules as illustrated in Figures **4.5** and **4.6**. The

variational transition states for the association of BH_3 with 3-methylcyclohexene to afford the π-complexes were located by an adaptation of the "nosaddle" procedure of Truhlar and coworkers[83,84]. The starting point for the location of **4e-23**‡ and **4e-24**‡ were the lowest-energy structures found in a scan of positions with BH_3 and 3-methylcyclohexene associated by separated by 5 Å (Table **4.14**). From these structures, with the program PROGDYN,[84] the steepest-descent paths in mass-weighted coordinates were followed in each case as described for other alkenes. The structures **4e-23**‡ and **4e-24**‡ were the free-energy maximum along these paths when the free energy is graph against the B-C1 and B-C2 distance.

Table 4.14. Calculated enthalpies and free energies for the variational transition state structures located for the reaction of BH_3 with 3-methylcyclohexene with the methyl in the equatorial position.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
4e-23‡	$\Delta G^{\ddagger} = 3.7$ $\Delta H^{\ddagger} = -4.0$	$\Delta G^{\ddagger} = 4.9$ $\Delta H^{\ddagger} = -3.8$	$\Delta G^{\ddagger} = 6.3$ $\Delta H^{\ddagger} = -2.8$
4e-24‡	$\Delta G^{\ddagger} = 3.8$ $\Delta H^{\ddagger} = -5.0$	$\Delta G^{\ddagger} = 5.2$ $\Delta H^{\ddagger} = -4.8$	$\Delta G^{\ddagger} = 6.8$ $\Delta H^{\ddagger} = -3.5$

Because variational transition states are more difficult to obtain a geometry optimization of the variational transition state was only carried out in one calculational method. The energies chosen for the discussion that follows are based on the G3B3 calculations. This choice is based on the various results observed in the propene

hydroboration study. In that case the G3B3 energy transition leading to the products Markovnikov and anti-Markovnikov were found to match quite closely with other high-level calculations, including CCSD(T) calculations employing very large basis sets. In the propene hydroboration case a more extensive computational work was straightforwardly done, including CCSD(T) with an extrapolated to infinite basis set. This was feasible due the reality that unlike in this system the computational power required was reasonable.

We were able to follow the free-energy alongside the reaction progress starting with separate starting materials. The starting materials lead to the variational transition states **4e-23**‡ and **4e-24**‡, and these lead **4e-3** and **4e-4.** From π-complex **4e-3** the two transition structures **4e-7**‡ and **4e-8**‡ lead to the regioisomeric products **4e-18** and **4e-15** respectively. The $\Delta\Delta G^{‡}$ for **4e-7**‡ and **4e-8**‡ was predicted to be 0.0 kcal/mol, of that no selectivity would be predicted between the two products. The barrier associated with these structures form the π-complex **4e-3** is 3.6 kcal/mol. Both structures are of course higher in potential energy than **4e-3**. In the case of **4e-24**‡ to form π-complex **4e-4** the two transition structures **4e-9**‡ and **4e-10**‡ lead to the regioisomeric products **4e-16** and **4e-17,** respectively.

The $\Delta\Delta G^{‡}$ for **4e-9**‡ versus **4e-10**‡ was predicted to be 0.0 kcal/mol. The barrier associated with these structures form the π-complex **4e-4** is 2.7 kcal/mol. No selectivity is predicted between the regiio isomeric product 4e-16 and 4e-17. The reaction coordinate diagram for these reactions involving they hydroboration of the equatorial methylcyclohexene as shown in Figure **4.6**.

We also predicted the energies of the cis and trans attack of the BH_3 to the 3-methylcyclohexene with the methyl on the axial position, structure **4e-2.** The reaction coordinate diagram for these pathways are illustrated in Figure **4.7**. Because the difficulty of calculating variational transition structures were located for the axial 3-methylcyclohexene reactions. The equatorial variational transition structures **4e-23**‡ and **4e-24**‡ are more likely to be the ones reacting in solution. The expected variational transition state energies for these reactions are positioned qualitatively in the reaction coordinate diagrams. Based on the energies for **4e-23**‡ and **4e-24**‡ this is likely an underestimate of the free energy of the variational transition states from BH_3 associated to 4e-2. Graph (a) in Figure **4.5** shows the pathway of the π-complex **4e-5** leads to the two transition structures **4e-11**‡ and **4e-12**‡. These transition structures lead to the regioisomeric products **4e-22** and **4e-19,** respectively. The $\Delta\Delta G^{‡}$ for **4e-11**‡ versus **4e-12**‡ was predicted to be 0.5 kcal/mol. The barriers associated with these structures from **4e-5** were 3.8 and 4.3 kcal/mol, repectively. Graph (b) illustrates the reaction coordinate diagram when the borane attacks the axial methylcyclohexene from the opposite face. This forms π-complex **4e-6.** Complex **4e-6** leads to two transition structures **4e-13**‡ and **4e-14**‡. These transition structures lead to the regioisomeric products **4e-20** and **4e-21,** respectively. The $\Delta\Delta G^{‡}$ for **4e-13**‡ and **4e-14**‡ was predicted to be 0.2 kcal/mol, the barrier associated with these structures from **4e-3** is between 1.4 and 1.6 kcal/mol, repectively. These approximations predict an experimental ratio representing no selectivity between C-1 and C-2 in any case. This is not in agreement with experimental

results. Importantly, no anharmonic correction has been considered for any or these predictions.

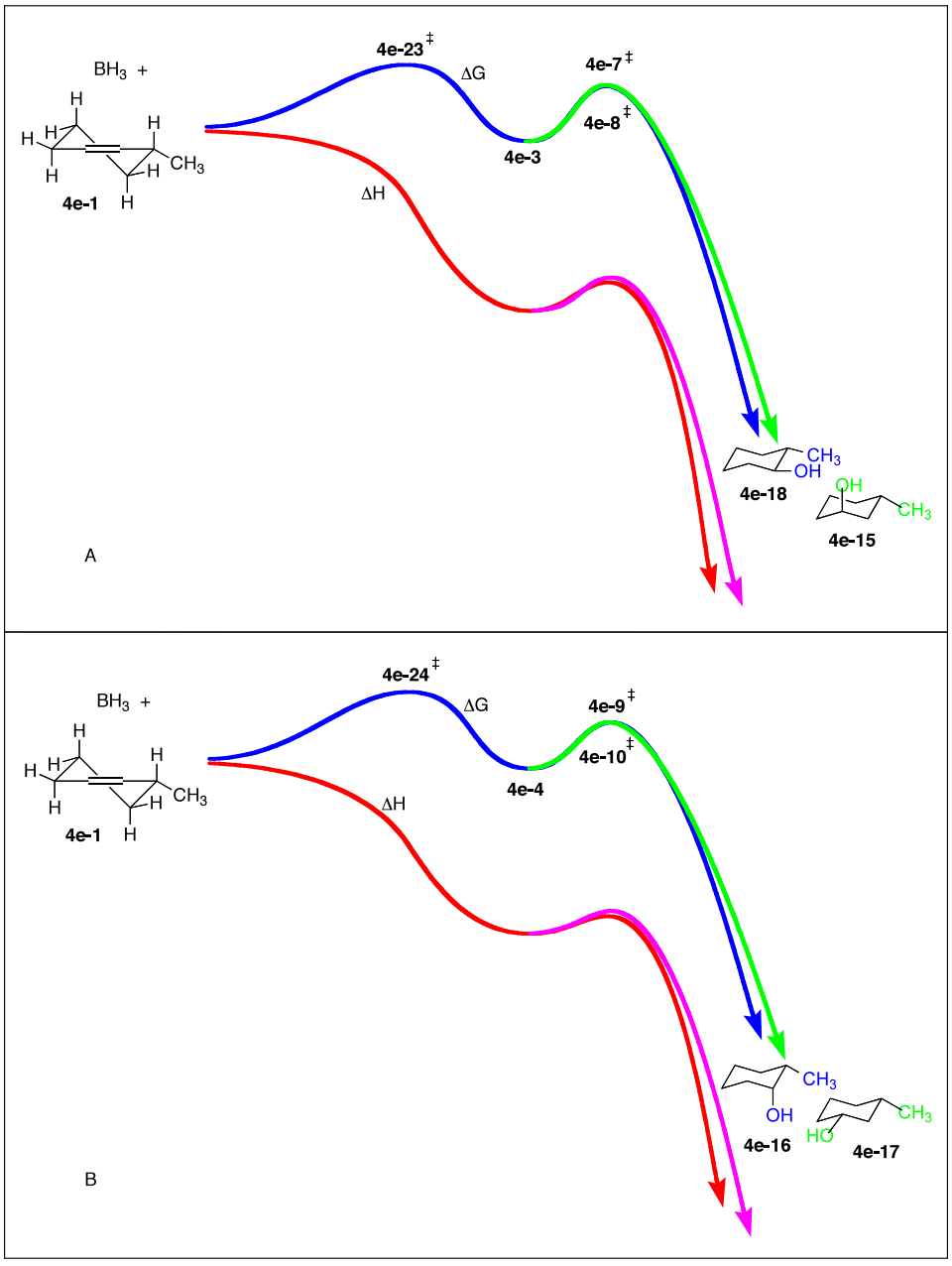


Figure 4.6. Reaction coordinate diagram for the hydroboration of equatorial 3-methylcyclohexene based on the predicted G3B3 enthalpies and free energies. (A) trans attack of the borane and (B) cis attack of the borane.

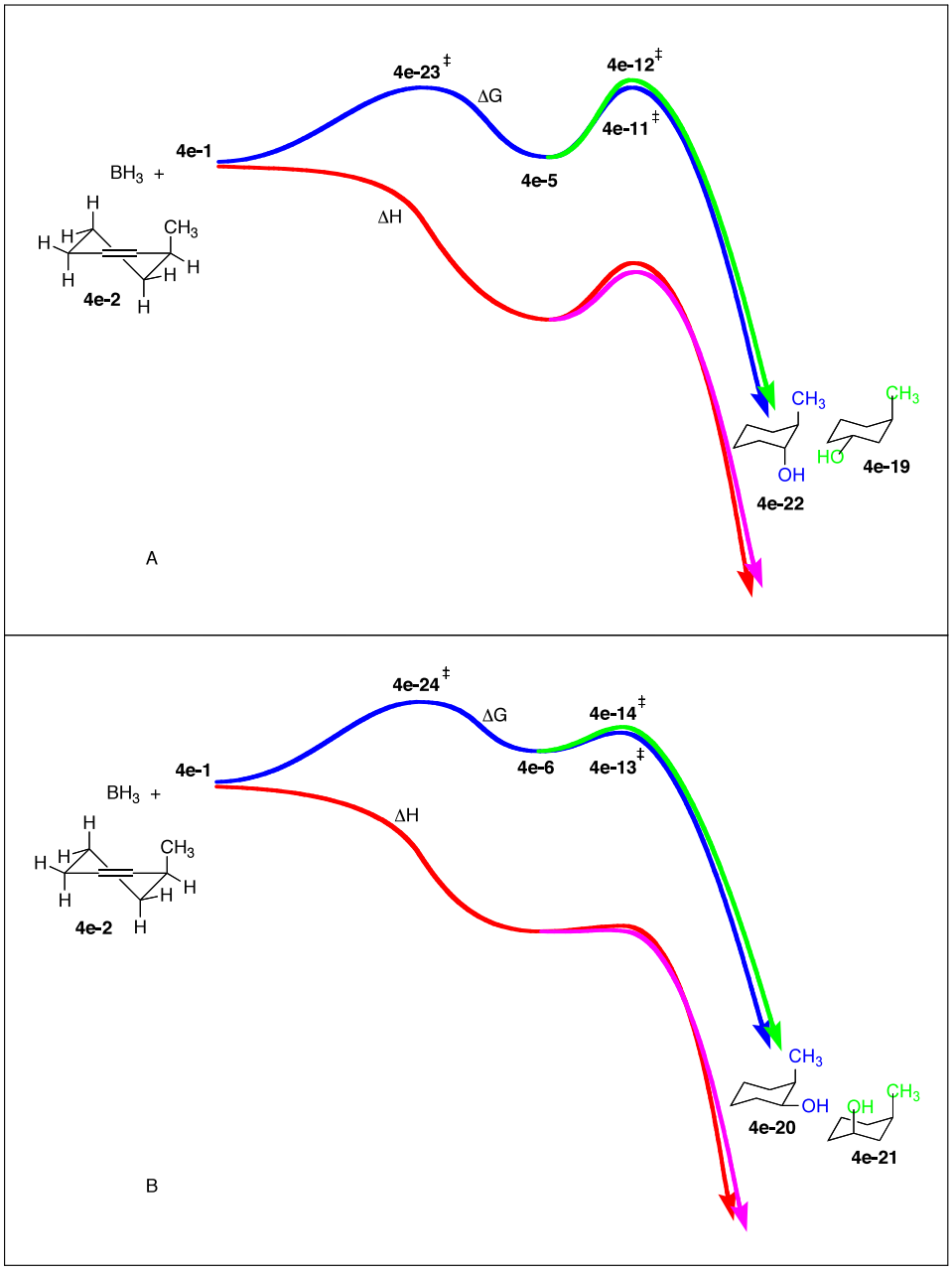


Figure 4.7. Reaction coordinate diagram for the hydroboration of axial 3-methylcyclohexene based on the predicted G3B3 enthalpies and free energies. (A) trans attack of the borane and (B) cis attack of the borane.

We hypothesize that the anharmonic correction of the energies found could give a more accurate approximation, which is expected to lead a truthful comparison of the

experimental and ratio calculated. We expect a significant impact from these corrections as we have already considered potential miscalculations in other hydroboration systems and we find second-order perturbative anharmonic contributions to the vibrational energies and entropy to impact the results due to the fact that we are predicting such small $\Delta\Delta G^{\ddagger}$. Also, other potential errors in the prediction of $\Delta\Delta G^{\ddagger}$ in the hydroboration of propene with BH_3 were considering, such as tunneling. Yet, in this case since the barrier associated between transition structures **4e-7**‡ and **4e-8**‡ was negligible, tunneling should contribute little to the rate of the anti-Markovnikov process. Any simple error of in the relative energies of the transition structures cannot be directly excluded.

We have calculated the contributions from the second-order perturbative anharmonic corrections to the vibrational energies and entropy to fix the predicted ΔG for all the barriers from π-complexes to all transition structures leading to any possible Markovnikov or anti-Markovnikov product relative to the corrected separate starting materials. The newly corrected prediction, expressed in kcal/mol, for starting material **4e-2** are listed on Table **4.8**, π-complexes **4e-3** to **4e-6** are reported on Table **4.15**, predictions for the transition structures **4e-7**‡ to **4e-10**‡ corresponding to the reaction of BH_3/3-methylcyclohexene with the methyl in the equatorial position and the transition structures **4e-11**‡ to **4e-14**‡, corresponding to the reaction of BH_3/3-methylcyclohexene with the methyl in the are depicted in Tables **4.16** and **4.17** respectively.

Table 4.15. Predicted free energy after anharmonic adjustment for all structures located for the complexes formed form combining BH_3 with 3-methylcyclohexene with the methyl in the axial position according to a variety of methods/basis set calculations, the energetics are relative to the starting material and expressed in kcal/mol.

Structure / Method / Basis Set	**4e-3**	**4e-4**	**4e-5**	**4e-6**
G3B3	ΔG = - 1.2	ΔG = -0.1	ΔG = - 1.6	ΔG = 0.48
B3LYP/6-31G*	ΔG = 2.5	ΔG = 5.4	ΔG = 2.3	ΔG = 4.48
B3LYP/6-31+G**	ΔG = 4.0	ΔG = 6.9	ΔG = 4.0	ΔG = 6.18
CBS-QB3	ΔG = - 0.9	ΔG = 3.7	ΔG = - 1.7	ΔG = 0.78
CCSD(T)/6-311+G**	ΔG = 3.0	ΔG = 3.3	ΔG = -1.2	ΔG = 1.08
CCSD(T/)6-31+G**	ΔG = 2.2	ΔG = 5.2	ΔG = 2.0	ΔG = 4.4
CCSD(T)/aug-cc-pvdz	ΔG = 2.6	ΔG = 2.8	ΔG = - 1.8	ΔG = 0.4
CCSD(T)/cc-pvdz	ΔG = 0.8	ΔG = 3.8	ΔG = -0.4	ΔG = 2.8

Table 4.15 continued.

Structure / Method / Basis Set	**4e-3**	**4e-4**	**4e-5**	**4e-6**
MO5/631+G**	ΔG = 1.4	ΔG = 3.9	ΔG = 1.6	ΔG = 3.0
MP4(sdq)/aug-cc-pvdz	ΔG = 7.3	ΔG = 10.2	ΔG = 7.1	ΔG = 9.2
MP4(sdtq)/cc-pvtz	ΔG = 0.2	ΔG = 3.1	ΔG = -0.1	ΔG = 2.1
B1B95/6-31+G**	ΔG = - 25	ΔG =0.3	ΔG = -2.3	ΔG = - -0.8
MPWLYP/6-31+G**	ΔG = 2.6	ΔG = 5.5	ΔG = 2.6	ΔG = 4.7
MPWPW91/6-31+G**	ΔG = - 1.5	ΔG = 1.2	ΔG = - 1.6	ΔG = 0.3
TPSSTPSS/cc-pvtz	ΔG = 42.9	ΔG = 45.8	ΔG = 43.0	ΔG = 44.9

Table 4.16. Calculated free energy after anharmonic adjustment for the transition state structures located for the reaction of BH_3 with 3-methylcyclohexene with the methyl in the equatorial position.

Structure / Method / Basis Set	**4e-7**	**4e-8**	**4e-9**	**4e-10**
G3B3	$\Delta G^{\ddagger}$ = 2.5	$\Delta G^{\ddagger}$ = 3.0	$\Delta G^{\ddagger}$ = 2.5	$\Delta G^{\ddagger}$ = 1.0
B3LYP/6-31G*	$\Delta G^{\ddagger}$ = 6.7	$\Delta G^{\ddagger}$ = 7.2	$\Delta G^{\ddagger}$ = 7.1	$\Delta G^{\ddagger}$ = 5.6
B3LYP/6-31+G**	$\Delta G^{\ddagger}$ = 7.7	$\Delta G^{\ddagger}$ = 8.2	$\Delta G^{\ddagger}$ = 8.2	$\Delta G^{\ddagger}$ = 6.8
CBS-QB3	$\Delta G^{\ddagger}$ = 2.9	$\Delta G^{\ddagger}$ = 3.4	$\Delta G^{\ddagger}$ = 3.0	$\Delta G^{\ddagger}$ = 1.8
CCSD(T)/6-311+G**	$\Delta G^{\ddagger}$ = 3.0	$\Delta G^{\ddagger}$ = 3.4	$\Delta G^{\ddagger}$ = 3.2	$\Delta G^{\ddagger}$ = 2.1
CCSD(T)/6-31+G**	ΔG = 6.1	ΔG = 6.5	ΔG = 6.3	ΔG = 5.2
CCSD(T)/aug-cc-pvdz	$\Delta G^{\ddagger}$ = 3.1	$\Delta G^{\ddagger}$ = 3.6	$\Delta G^{\ddagger}$ = 3.4	$\Delta G^{\ddagger}$ = 2.0
CCSD(T)/cc-pvdz	$\Delta G^{\ddagger}$ = 4.8	$\Delta G^{\ddagger}$ = 5.3	$\Delta G^{\ddagger}$ = 5.15	$\Delta G^{\ddagger}$ = 3.8

Table 4.16 continued.

Structure / Method / Basis Set	**4e-7**	**4e-8**	**4e-9**	**4e-10**
MO5/631+G**	$\Delta G^{\ddagger}$ = 0.2	$\Delta G^{\ddagger}$ = 0.6	$\Delta G^{\ddagger}$ = 0.4	$\Delta G^{\ddagger}$ = -0.7
MP4(sdq)/aug-cc-pvdz	$\Delta G^{\ddagger}$ = 5.1	$\Delta G^{\ddagger}$ = 5.6	$\Delta G^{\ddagger}$ = 5.4	$\Delta G^{\ddagger}$ = 4.0
MP4(sdtq)/cc-pvtz	$\Delta G^{\ddagger}$ = 3.8	$\Delta G^{\ddagger}$ = 4.7	$\Delta G^{\ddagger}$ = 4.0	$\Delta G^{\ddagger}$ = 2.8
B1B95/6-31+G**	$\Delta G^{\ddagger}$ = - 1.1	$\Delta G^{\ddagger}$ = - 1.7	$\Delta G^{\ddagger}$ = - 1.2	$\Delta G^{\ddagger}$ = - 0.1
MPWLYP/6-31+G**	$\Delta G^{\ddagger}$ = 6.2	$\Delta G^{\ddagger}$ = 6.8	$\Delta G^{\ddagger}$ = 3.6	$\Delta G^{\ddagger}$ = 5.3
MPWPW91/6-31+G**	$\Delta G^{\ddagger}$ = - 0.3	$\Delta G^{\ddagger}$ = - 0.5	$\Delta G^{\ddagger}$ = - 0.1	$\Delta G^{\ddagger}$ = -1.3
TPSSTPSS/cc-pvtz	$\Delta G^{\ddagger}$ = 46.0	$\Delta G^{\ddagger}$ = 46.7	$\Delta G^{\ddagger}$ = 46.6	$\Delta G^{\ddagger}$ = 45.3

Table 4.17. Calculated free energy after anharmonic adjustment for the transition state structures located for the reaction of BH_3 with 3-methylcyclohexene with the methyl in the axial position.

Structure / Method / Basis Set	**4e-11**	**4e-12**	**4e-13**	**4e-14**
G3B3	$\Delta G^{\ddagger}$ = 3.63	$\Delta G^{\ddagger}$ = 4.2	$\Delta G^{\ddagger}$ = 2.7	$\Delta G^{\ddagger}$ = 2.8
B3LYP/6-31G*	$\Delta G^{\ddagger}$ = 8.13	$\Delta G^{\ddagger}$ = 8.5	$\Delta G^{\ddagger}$ = 8.9	$\Delta G^{\ddagger}$ = 8.7
B3LYP/6-31+G**	$\Delta G^{\ddagger}$ = 9.23	$\Delta G^{\ddagger}$ = 9.7	$\Delta G^{\ddagger}$ = 10.1	$\Delta G^{\ddagger}$ = 1.0
CBS-QB3	$\Delta G^{\ddagger}$ = 3.93	$\Delta G^{\ddagger}$ = 4.5	$\Delta G^{\ddagger}$ = 4.7	$\Delta G^{\ddagger}$ = 4.5
CCSD(T)/6-311+G**	$\Delta G^{\ddagger}$ = 4.13	$\Delta G^{\ddagger}$ = 4.7	$\Delta G^{\ddagger}$ = 5.0	$\Delta G^{\ddagger}$ = 4.9
CCSD(T)/6-31+G**	$\Delta G^{\ddagger}$ = 7.7	$\Delta G^{\ddagger}$ = 7.9	$\Delta G^{\ddagger}$ = 8.3	$\Delta G^{\ddagger}$ = 8.1
CCSD(T)/aug-cc-pvdz	$\Delta G^{\ddagger}$ = 4.3	$\Delta G^{\ddagger}$ = 4.7	$\Delta G^{\ddagger}$ = 4.86	$\Delta G^{\ddagger}$ = 4.7
CCSD(T)/cc-pvdz	$\Delta G^{\ddagger}$ = 6.0	$\Delta G^{\ddagger}$ = 6.5	$\Delta G^{\ddagger}$ = 6.8	$\Delta G^{\ddagger}$ = 6.6

Table 4.17 continued.

Structure / Method / Basis Set	**4e-11**	**4e-12**	**4e-13**	**4e-14**
MO5/631+G**	$\Delta G^{\ddagger}$= 1.5	$\Delta G^{\ddagger}$= 2.0	$\Delta G^{\ddagger}$= 2.4	$\Delta G^{\ddagger}$= 2.3
MP4(sdq)/aug-cc-pvdz	$\Delta G^{\ddagger}$= 6.3	$\Delta G^{\ddagger}$= 6.8	$\Delta G^{\ddagger}$= 7.0	$\Delta G^{\ddagger}$= 6.8
MP4(sdtq)/cc-pvtz	$\Delta G^{\ddagger}$= 5.0	$\Delta G^{\ddagger}$= 5.5	$\Delta G^{\ddagger}$= 5.8	$\Delta G^{\ddagger}$= 5.6
B1B95/6-31+G**	$\Delta G^{\ddagger}$= - 0.1	$\Delta G^{\ddagger}$= 0.2	$\Delta G^{\ddagger}$= 0.5	$\Delta G^{\ddagger}$= 0.5
MPWLYP/6-31+G**	$\Delta G^{\ddagger}$= 7.7	$\Delta G^{\ddagger}$= 8.2	$\Delta G^{\ddagger}$= 8.5	$\Delta G^{\ddagger}$= 8.4
MPWPW91/6-31+G**	$\Delta G^{\ddagger}$= 0.9	$\Delta G^{\ddagger}$= 1.4	$\Delta G^{\ddagger}$= 1.9	$\Delta G^{\ddagger}$= 1.6
TPSSTPSS/cc-pvtz	$\Delta G^{\ddagger}$= 47.4	$\Delta G^{\ddagger}$= 48.0	$\Delta G^{\ddagger}$= 48.2	$\Delta G^{\ddagger}$= 48.0

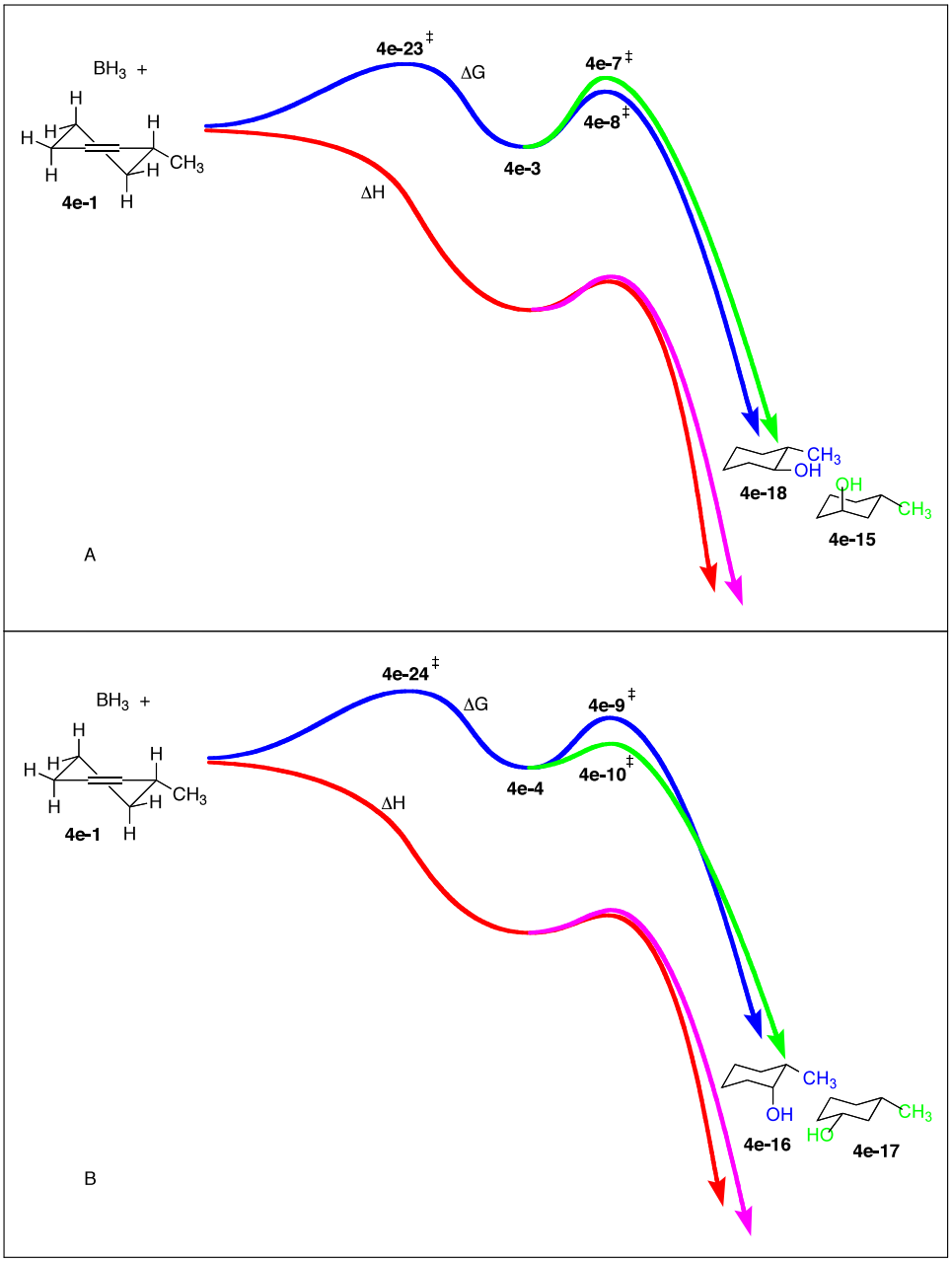


Figure 4.8. Reaction coordinate diagram for the hydroboration of equitorial 3-methylcyclohexene based on the predicted G3B3 enthalpies and free energies after anharmonic corrections. (A) trans attack of the borane and (B) cis attack of the borane.

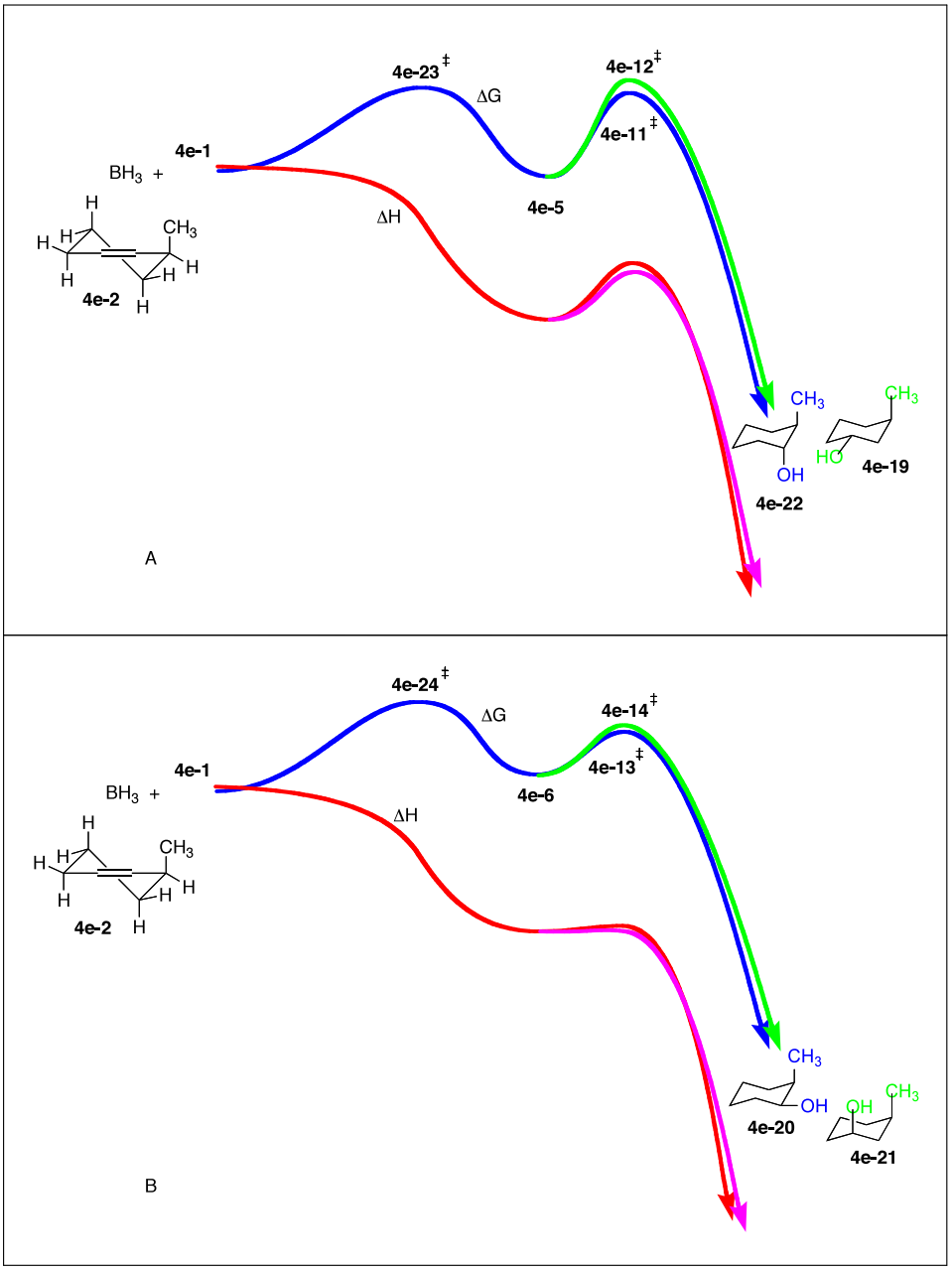


Figure 4.9. Reaction coordinate diagram for the hydroboration of axial 3-methylcyclohexene based on the predicted G3B3 enthalpies and free energies after anharmonic corrections. (A) trans attack of the borane and (B) cis attack of the borane.

Having properly allowed for the anharmonic adjustment we were able to establish theoretical energy differences for contrast against experimental. Restructuring, all over again, the free-energy alongside the reaction progress starting with separate starting material but now with the rationalized energies after the tuning are represented in Figures **4.8** and **4.9**. Figure **4.8**-a illustrates the reaction of BH_3 approaching the 3-methylcyclohexene *trans* to the methyl in the equatorial position. The initial barriers **4e-23**‡ and **4e-24**‡ to form **4e-3** and **4e-4** have not been changed**.** Now from π-complex **4e-3** the two transition structures **4e-7**‡ and **4e-8**‡ lead to the regioisomeric products **4e-18** and **4e-15** respectively the barrier is calculated to be 3.8 and 4.2 kcal/mol correspondingly. The $\Delta\Delta G^{‡}$ for **4e-7**‡ and **4e-8**‡ was corrected to be 0.4 kcal/mol, this will theoretically represent a selectivity of 34:66 of **4e-8**‡ and **4e-7**‡. Both structures are of course still higher in potential energy than **4e-3**. In the case of Figure **4.8**-b, the reaction of BH_3 approaching the 3-methylcyclohexene *cis* to the methyl in the equatorial, the position **4e-24**‡ to form π-complex **4e-4** was not changed. For the two transition structures **4e-9**‡ and **4e-10**‡ leading to the regioisomeric products **4e-16** and **4e-17** the barriers were 2.4 and 0.9 kcal/mol from π-complex **4e-4**. The $\Delta\Delta G^{‡}$ for **4e-9**‡ and **4e-10**‡ was corrected to be 1.4 kcal/mol, the ratio expected experimentally, according to this difference in energy will be in theory 9:91 of **4e-10**‡ and **4e-9**‡.

As shown in Figure **4.9**, we also predicted the energies of the cis and trans attack of the BH_3 to the 3-methylcyclohexene with the methyl on the axial position, structure **4e-2** after corrections. However, as in the other cases, only the variational transition structures that were more likely be the ones reacting in solution, the variational transition

structures **4e-23**‡ and **4e-24**‡, corresponding to the cis and trans association of BH_3 and 3-methylcyclohexene with the methyl on the equatorial position (**4e-1)**, were located due to the time consuming process in locating these structures. Nonetheless we decided to position the more stable corresponding variational transition structures to help visualize a complete reaction coordinate for these cases, as this is an underestimate of the free energy of the variational transition states from BH_3 associated to **4e-2**. Figure **4.9** represents π-complex **4e-5** the two transition structures **4e-11**‡ and **4e-12**‡ lead to the regioisomeric products **4e-22** and **4e-19** respectively after the anharmonic adjustments. The $\Delta\Delta G^{‡}$ for **4e-11**‡ and **4e-12**‡ was predicted, after adjustments, to be 0.6 kcal/mol, for such a small difference in energy the experimental selectivity expected for **4e-12**‡ and **4e-11**‡ will be close to 27:73. The barriers associated with these structures form **4e-5** are now 5.2 and 5.8 kcal/mol. In the case of graph b in Figure **4.9**, form π-complex **4e-6** the two transition structures **4e-13**‡ and **4e-14**‡ lead to the regioisomeric products **4e-20** and **4e-21**, the $\Delta\Delta G^{‡}$ for **4e-13**‡ and **4e-14**‡ was calculated to be 0.1 kcal/mol, in other words the ratio calculated for **4e-14**‡ and **4e-13**‡ approximates a mixture of 45.5:54.5. The barriers associated with these structures form **4e-3** are approximately 2.2 and 2.3 kcal/mol.

We make out that in each and every one of the approximations for $\Delta\Delta Gs^{‡}$ show the barrier for the formation of the C-2 product as lower in energy, experimentally this would predicts a ratio representing a preference in selectivity for C-2 over C-1 in every case, which is not always true for the experimental results obtained. Experimentally, C-2 was determined to be the preferred product but only in the case of the trans attack of the

BH_3, which leads to the transition structure **4e-7**‡. On the other hand, every experiment performed by Brown as well as our results point at product **4e-16**, formed from transition state **4e-9**‡, was the least selective. This implicated that transition state theory is not adequate to predict the regioselectivity between C1 and C2 in the hydroboration of 3-methylcyclohexene with BH_3.

When compared the stability of products does not match the experimental mixture of products. Products **4e-15** and **4e-17** were obtained approximately equally experimentally. Computationally, **4e-18** was found lowest in energy and very close in energy to **4e-16, 4e-18** were **4e-16** is the least favored experimentally. Yet, the lowest energy transition state was **4e-10**‡, which leads to product **4e-17**. The comparison of products afforded by the reactions performed and the stability of the free energy of the products were not in agreement. As a result, the experimental regioselectivity observed was not a consequence of the stability of the products.

We proposed the hydroboration of 3-methylcyclohexene with BH_3 to be a case of dynamics. Where the association barriers, the variational transition structures **4e-23**‡ and **4e-24**‡, may cause the formation of π-complexes to provide considerable excess energy. Thus excess energy is available for π-complex to pass to product faster that thermal equilibration with solvent. From this idea we decided to perform dynamic trajectories from the variational transition structures **4e-23**‡ and **4e-24**‡. Trajectories started from **4e-23**‡, did not afforded many products after 5000 fs. From 45 trajectories, 14 bounced back to starting material, 29 stayed equilibrating close to the π-complex **4e-3** and 2 formed product. The product formed corresponded to the product from the C-2 attack, product

4e-18 from transition state **4e-7**‡. We explore a series of classical trajectory form variational transition structure **4e-24**‡ and they were slightly more successful after 5000 fs than trajectories form variational transition structure **4e-23**‡. From 93 trajectories, 24 bounced back to starting material, 55 stayed equilibrating nearby the π-complex **4e-4** and 10 trajectories formed product. The products formed corresponded to a ratio of products of 10:4 from the C-2 attack and the C-1 attack respectively, which are products **4e-16** and **4e-17**. At this point an initial tendency was observed a preference for the formation of product from the C-2 attack of the BH_3 in agreement with the energetics calculated. Although the fact that initial tendencies are in agreement is not indicative that the inclination will be the same if more trajectories were consider.

More dynamic trajectories required to determine if concrete prediction of the regioselectivity in this case and to conclude it these will be in agreement with the experimental ratio of products. An influential amount of trajectories were reached due to the fact that the barriers for the formation of product are large translating in a more time consuming task. This is due the reality that unlike in other previously discussed systems the computational power required was unreasonable.

Despite this, we conclude that in this case transition state theory is not able to account for the ratio of products afforded experimentally. We strongly believe this is a case of dynamics.

Overall, for the hydroboration of internal disubstituted and trisubstituted alkenes we found an entropic association barrier for the formation of π-complex in all cases. It was determine for the internal disubstituted and trisubstituted alkenes that the formation

of such π-complex is enthalpically barrierless. Dynamics cases were establish, when the enthalpic association barrier found was the rate-limiting step and the barrier for the formation of products form π -complex were small. Various isotope effects were determined. These isotope effects were too small for the conventional mechanism to be the predominate pathway.

CHAPTER V

DYNAMICS AND SELECTIVITY IN THE HYDROBORATION OF ALKENES *VIA* CHLOROBORANE

Introduction

The hydroboration reaction between olefins and borane has proven to be a highly successful method for obtaining organoboranes. These can then be used as intermediates in the synthesis of a variety of materials. As previously established in Chapter I, when borane is used as a hydroborating agent, a product mixture of regioisomers is obtained but the use of monochloroboranes improves the selectivity for the formation of the anti-Markovnikov product to more than 99.5% isomeric purity.[34,91]

Brown first synthesized both mono- and dichloroborane etherates with sodium borohydride and boron trichloride (1:1) in a diglyme solution.[92] However, in the absence of ethers such as dimethyl ether, diethyl ether, diglyme, tetrahydrofuran, and tetrahydropyran, no reaction occurs.[92b] Onak *et al.* reacted diborane, boron trichloride and ether in stoichiometric amounts to form dichloroborane etherates. Lynds and Stern synthesized dichloroborane by passing H_2 and boron trichloride over granular magnesium at 400-450 °C.[38] It was shown a reaction between diborane with HCl[93]. This reaction proceeded very slow at room temperature, yet studies showed that the addition of diethyl ether[93b] greatly accelerated the formation of monochloroborane (2:1 molar ratio of HCl to B_2H_6).

Zweifel reported one of the first studies involving monochloroborane or dichloroborane as a reagent for the hydroboration reaction.[33b] Despite being slow compared to other hydroboration agents (e.g. BH_3, Thexyl-BH_2, and Sia_2BH) reactions using monochloroborane or dichloroboranes proved to be highly selective in obtaining the anti-Markovnikov product with up to 99% selectivity. It was speculated that the low reactivity of the chloroboranes might be a result of the formation of a complex with the solvent that effectively reduces the electrophilic character of the borane.

Research done by Lynds and Stern claimed that reactions involving dichloroborane and ethylene, propylene, isobutylene, or cyclohexene display a preference for the addition of the boron to the most substituted carbon forming the Markovnikov product.[38] On the other hand, Shchegoleva and co-workers proposed that when monochloroborane was used the anti-Markovnikov product was preferred.[94]

Pasto later investigated the reaction of mono- and dichloroboranes with 2-methylpropene, 1-hexene, and styrene in tetrahydrofuran and concluded that the addition of boron preferred the least substituted carbon-atom.[20b,33a] It was concluded form ^{1}H-NMR studies that the tetrahydrofuran solvent interacts strongly with monochloroborane, reducing its electrophilic nature, and diminishes its reactivity.

Pasto investigated the reaction further by examining plots of log *k vs.* σ and σ^+ and found that σ produced ρ values of -0.65 for internal and -1.43 for terminal addition respectively; further supporting the idea that tetrahydrofuran complexes with chloroborane.[20b] Interestingly, the effects look small in most substitutions, only NO_2 seem to have lower selectivity. Kinetic isotope effects were also measured to give k_H/k_D

values of 2.4 for 1-hexene, 1.78 and 1.87 for styrene (25 °), and 1.56 and 1.68 for styrene (35 °C). Pasto attributed the k_H/k_D isotope effect results to Brown's proposal that a four-centered transition state is formed for the hydroboration of olefins with monochloroborane, rejecting the alternative proposal from Streitwieser (a triangular π-complex that slightly shifted into a transition state).

The hydroboration of olefins using monochloroborane and dichloroborane mentioned thus far have only been carried out in basic solvents such as tetrahydrofuran. The complex formed reduces the electrophilic character of the chloroboranes making the hydroboration reaction proceed slowly. Brown investigated the possibility of using less basic solvents to reduce the interaction of the chloroboranes with the solvent in hopes of increasing the reaction rate.[34] When diethyl ether was used as solvent, since it is less basic, the rate of reaction was determined to be 2 mol of olefin/mol of BH_2Cl per hour while in the case of cyclohexene and styrene the reaction proceeded at 2 mol of olefin/mol of BH_2Cl at 2 and 16 hours. Not only did performing the hydroboration reaction of olefins with monochloroborane in the presence of ethyl ether increase the rate of reaction, but it also greatly enhanced selectivity for the anti-Markovnikov product.[91a] Previous reports indicate that monochloroborane in THF showed a 94:6 product distribution in the hydroboration of 1-hexene to 1-hexanol and 2-hexanol, this result will be discussed again later.[33a,93c] The reactions of olefins with dichloroborane were found to be very slow in tetrahydrofuran due to the strong complexation effects. When BCl_3 in pentane was added to the reaction mixture the reaction went to completion within minutes and proved to be applicable to a wide range of alkenes.[37]

Brown additionally discovered that monochloroborane in dioxane was a highly reactive hydroborating agent with high preferences for the formation of the anti-Markovnikov product.[35a] The monochloroborane-dioxane complex was capable of hydroborating monosubstituted, disubstituted, and trisubstituted olefins very rapidly into dialkylchloroboranes. A series of Lewis bases including, tert-butyl methyl ether, dioxane, anisole, ethyl acetate, β-chloroethyl ether, and monoglyme were studied as solvents for the hydroboration with BH_2Cl and $BHCl_2$; however, dioxane proved to be the most effective. It was determined that monochloroborane in dioxane was the most reactive giving nearly pure (>99.5%) of the primary alcohol. The advantage that the chloroboranes (especially monochloroborane) offers is that nearly pure products can be obtained and this simplifies the separation purification step that is often difficult.

In general, the experimental regioselectivity of monochloroborane and dichloroborane is modest to good, giving preferentially the anti-Markovnikov product. This observed regioselectivity has traditionally been explained by transition state theory. However, it should be of considerable interest to explore the degree to which dynamic effect can be brought in to explain the selectivity of the reaction with these alternative hydroboration agents. Our strategy, as in the previous cases, will be to determine the $\Delta\Delta G^{\ddagger}$ computationally from the transition states leading to regioisomeric products to compare with the experimental $\Delta\Delta G^{\ddagger}$.

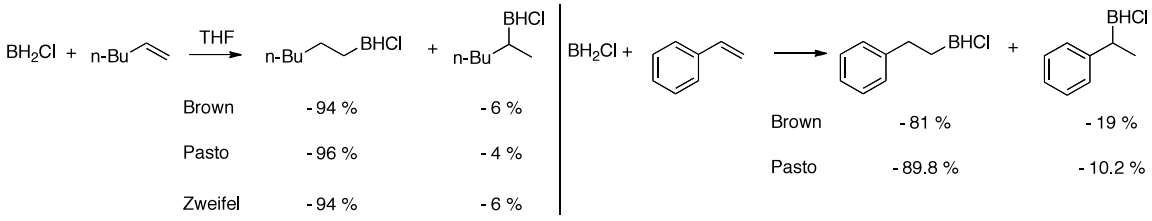
In order to do this we will refer to energies obtained by the composite method G3B3. As explained earlier, G3B3 energies perform as one of the best compared to

CCSD(T)/aug-cc-pvqz calculations and the difference in the energetics stayed within 0.1 kcal/mol.

Hydroboration of Alkenes with BH_2Cl

Interestingly, monochloroborane exists as a monomer in tetrahydrofuran and has been shown to be more electrophilic than borane.[20b] For this reason it is more acidic and is able to complex with the solvent (THF, SMe_2, OEt_2, dioxane) much stronger, which justifed why the rate of the reaction is decreased.[31] As we mentioned, Brown reported that the reaction with BH_2Cl in ethyl ether was more selective than BH_3 in THF; in the case of 1-hexene the product ratio was 99.5:0.5 1-hexanol to 2-hexanol.[36] On the other hand, Pasto, Brown and Zweifel reported ratios, in THF, of 96:4, 94:6 and 94:6 for 1-hexanol to 2-hexanol respectively for monochloroborane. These reported ratios are analogous to borane selectivity.[33,95]

Scheme 5.1

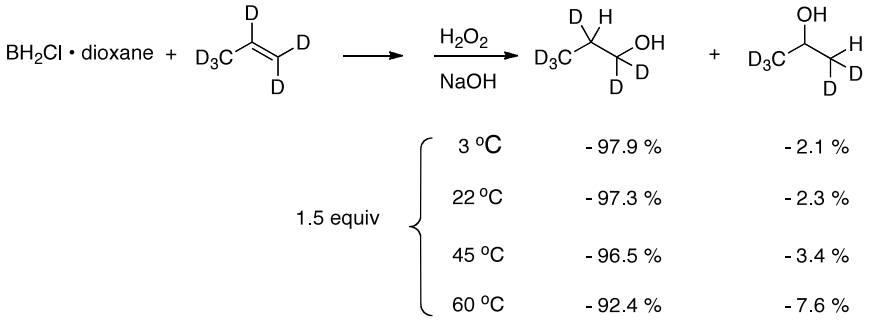


BH_2Cl•L (L=dioxane, SMe_2, OEt_2) when reacted with 1-hexene or styrene was found to be unexpectedly selective; the published ratio was ≈99.5:0.5 for 1-hexanol to 2-hexanol and ≈96:4 for 2-phenylethanol to 1-phenylethanol.[35,91b] The four-centered

transition state proposed by Brown is used to support the results, and it described as having a small charge being generated on the two carbons of the olefin.[26] The product was analyzed to determine if the dialkylcloroborane was formed when adding either together with one or two equivalents of alkene. The monoalkylchloroborane was the sole product detected by ^{11}B NMR spectroscopy in these reactions.

When we hydroborated propene-d_6 with BH_2Cl•L (L= SMe_2, dioxane), we found that the reaction was more selective than some previously reported. The propene-d_6 allowed us to directly measure the selectivity by ^2H-NMR. No purification was required, however, in some cases the layers in the mixture separated and additional water or methanol was needed in order to homogenize the solution.

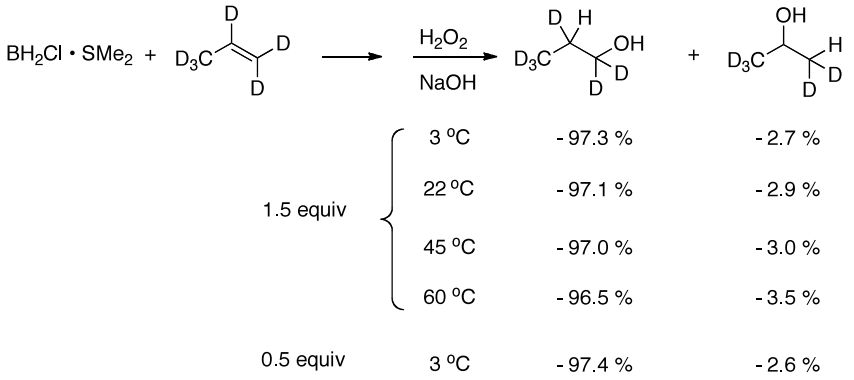
Scheme 5.2



We observed that when coordinated to SMe_2 the selectivity of the hydroboration is only slightly worse than when it was coordinated to dioxane at 22 ºC. Nonetheless, when BH_2Cl•SMe_2 was reacted with propene at high temperatures (45 ºC and 60 ºC) better selectivity was achieved than in the case of BH_2Cl in dioxane. These observations of small regioselectivity differences at different temperatures might be interpreted by the

potential for varying contributions from reactions of alkylboranes or dialkylboranes. The solvent polarity has no discernable effect on the regioselectivity.[67] Another possibility is the mechanistic complication of a direct transfer of the BH_3 from the solvent as ligand.

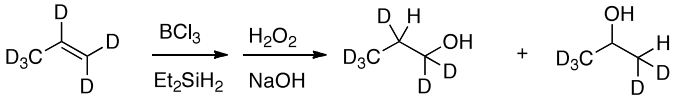
Scheme 5.3



When the monochloroborane is generated in situ by mixing BCl_3 with diethylsilane and propene-d_6 the selectivity at 22 ºC is not far from that of the coordinated borane. On the other hand, when excess of trichloroborane and diethylsilane versus alkene was added, the selectivity for the preferred anti-Markovnikov product lowered from 97.3% to 95.6%.

After determining the experimental regioselectivity for the hydroboration of simple alkenes with BH_2Cl, we considered whether transition state theory could accurately predict the observed selectivities.

Scheme 5.4



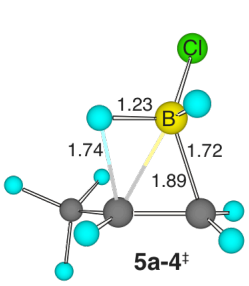
0.5 equiv	- 97.3 %	- 2.3 %
excess	- 95.6 %	- 4.4 %

Table 5.1. Enthalpies and free energies of structures located for the hydroboration of propene with BH_2Cl.

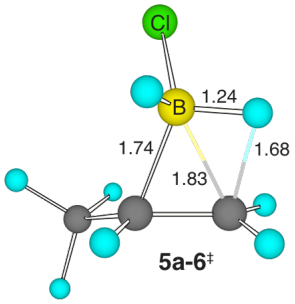
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
5a-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
5a-2	$\Delta G = 7.1$ $\Delta H = -3.6$	$\Delta G = 9.5$ $\Delta H = -3.3$	$\Delta G = 11.5$ $\Delta H = -1.4$
5a-3	$\Delta G = 7.2$ $\Delta H = -3.8$	$\Delta G = 9.6$ $\Delta H = -3.7$	$\Delta G = 11.5$ $\Delta H = -1.9$
5a-4‡	$\Delta G^{\ddagger} = 10.5$ $\Delta H^{\ddagger} = -2.1$	$\Delta G^{\ddagger} = 15.3$ $\Delta H^{\ddagger} = 1.5$	$\Delta G^{\ddagger} = 14.3$ $\Delta H^{\ddagger} = 0.3$
5a-5‡	$\Delta G^{\ddagger} = 10.5$ $\Delta H^{\ddagger} = -2.0$	$\Delta G^{\ddagger} = 15.6$ $\Delta H^{\ddagger} = 1.9$	$\Delta G^{\ddagger} = 14.0$ $\Delta H^{\ddagger} = 0.1$
5a-6‡	$\Delta G^{\ddagger} = 13.7$ $\Delta H^{\ddagger} = 1.2$	$\Delta G^{\ddagger} = 18.7$ $\Delta H^{\ddagger} = 4.4$	$\Delta G^{\ddagger} = 18.0$ $\Delta H^{\ddagger} = 4.0$
5a-7‡	$\Delta G^{\ddagger} = 13.0$ $\Delta H^{\ddagger} = 0.5$	$\Delta G^{\ddagger} = 17.8$ $\Delta H^{\ddagger} = 3.7$	$\Delta G^{\ddagger} = 16.8$ $\Delta H^{\ddagger} = 2.9$

Table 5.1 continued.

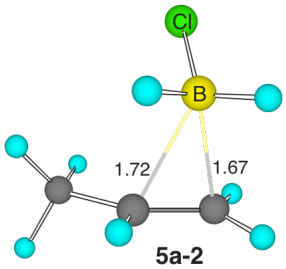
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
5a-8‡	$\Delta G^{\ddagger}$ = 5.6 $\Delta H^{\ddagger}$ = - 1.5	$\Delta G^{\ddagger}$ = 6.4 $\Delta H^{\ddagger}$ = - 1.5	$\Delta G^{\ddagger}$ = 7.3 $\Delta H^{\ddagger}$ = - 0.7
5a-9‡	$\Delta G^{\ddagger}$ = 5.9 $\Delta H^{\ddagger}$ = - 2.0	$\Delta G^{\ddagger}$ = 6.8 $\Delta H^{\ddagger}$ = - 1.9	$\Delta G^{\ddagger}$ = 7.8 $\Delta H^{\ddagger}$ = - 0.9
5a-10	ΔG = - 20.3 ΔH = - 31.2	ΔG = - 18.2 ΔH = - 32.5	ΔG = - 16.5 ΔH = - 30.8
5a-11	ΔG = - 19.9 ΔH = - 30.4	ΔG = - 18.2 ΔH = - 32.2	ΔG = - 15.6 ΔH = - 30.5
5a-12	ΔG = - 19.4 ΔH = - 30.2	ΔG = - 16.5 ΔH = - 30.7	ΔG = - 14.6 ΔH = - 28.8



5a-4‡



5a-6‡



5a-2

The transition structures leading to the regioisomeric products in the hydroboration of propene with BH_2Cl, structures **5a-4**‡, **5a-5**‡, **5a-6**‡ and **5a-7**‡, were located using B3LYP/6-31G* and B3LYP/6-31+G** calculations, in order to determine if the predicted $\Delta\Delta G^{\ddagger}$ corresponds to the experimental results. Structures **5a-4**‡ and **5a-5**‡

correspond to the barrier for the formation of the anti-Markovnikov product with the chlorine atom in different positions. Structures **5a-6**‡ and **5a-7**‡ correspond to the barrier for the formation of the Markovnikov product with the chlorine atom in possibly two different positions. The G3B3 $\Delta\Delta G^{‡}$ between **5a-4**‡ and **5a-6**‡ is 3.2 kcal/mol and between **5a-5**‡ and **5a-7**‡ is 3.0 kcal/mol. This translates to a predicted selectivity of ~99.3:0.7 for the anti-Markovnikov (**5a-10** and **5a-11**) to Markovnikov products (**5a-12**). The energies for all the structures located for the hydroboration of propene with BH_2Cl are contained in Table **5.1**.

From the determined $\Delta\Delta G^{‡}$, we can conclude that the experimental selectivity is less than the ratio predicted assuming that separate ratio of products observed arises from separate transition states energies leading to each products. Due to this fact, it is worth exploring if an entropic barrier might be involved in the hydroboration of simple alkenes with BH_2Cl.

An entropic association barrier located the variational transition structures **5a-8**‡ and **5a-9**‡, which corresponds to the free energy maximum along the steepest-descent path obtained using a modified version of PROGDYN. The difference between variational transition structures **5a-8**‡ and **5a-9**‡ is that the BH_2Cl ether approaches the propene or approaches the position of the chlorine atom in the structure. These were the lowest-energy structures found in a re-optimization of the π-complexes, structures **5a-2** and **5a-3**, which located positions with BH_2Cl and propene centroids separated by 5 Å. The G3B3 free energy barriers, from separate starting material to π-complexes **5a-2** and **5a-3**, are only 5.6 and 5.9 kcal/mol for **5a-8**‡ and **5a-9**‡ respectively.

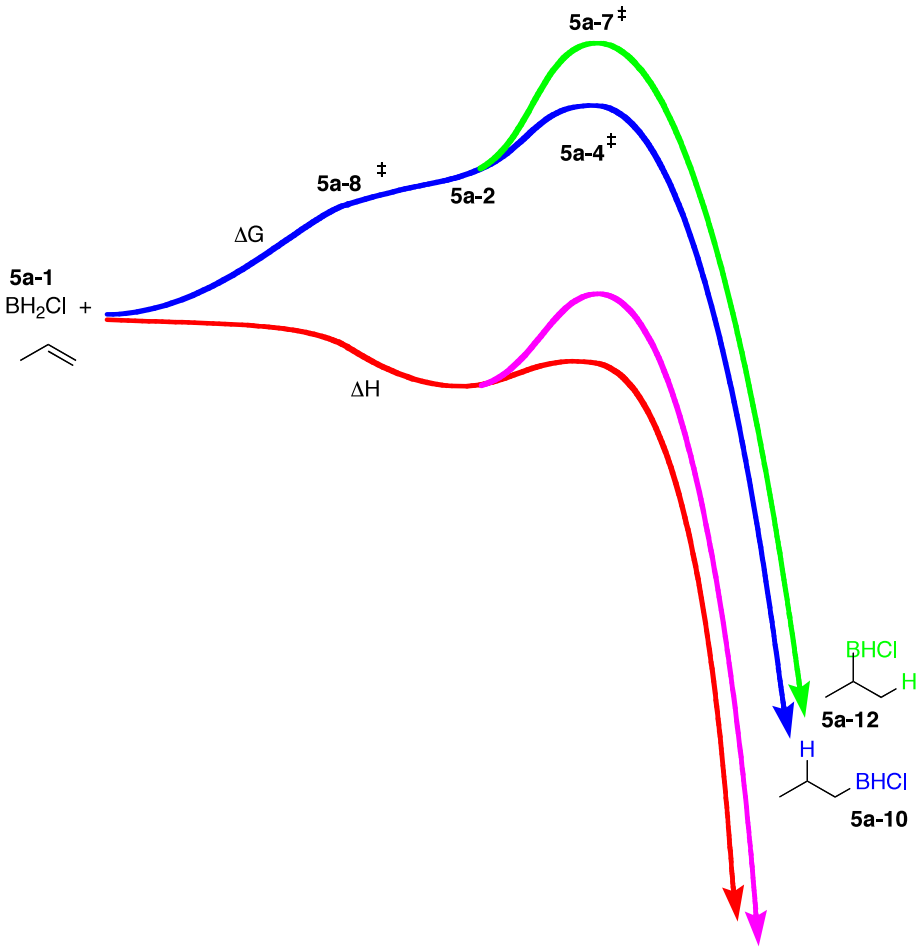
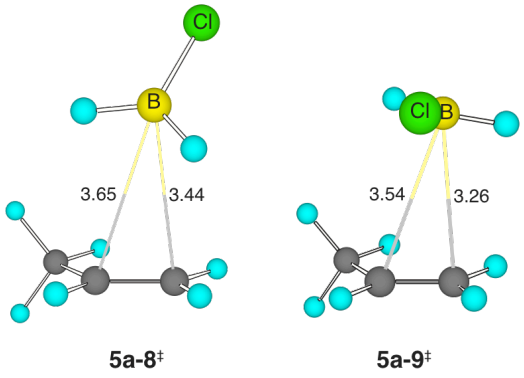


Figure 5.1. G3B3, ΔH and ΔG reaction coordinate diagrams for the lowest energy conformation structures located for the hydroboration of propene with BH_2Cl.



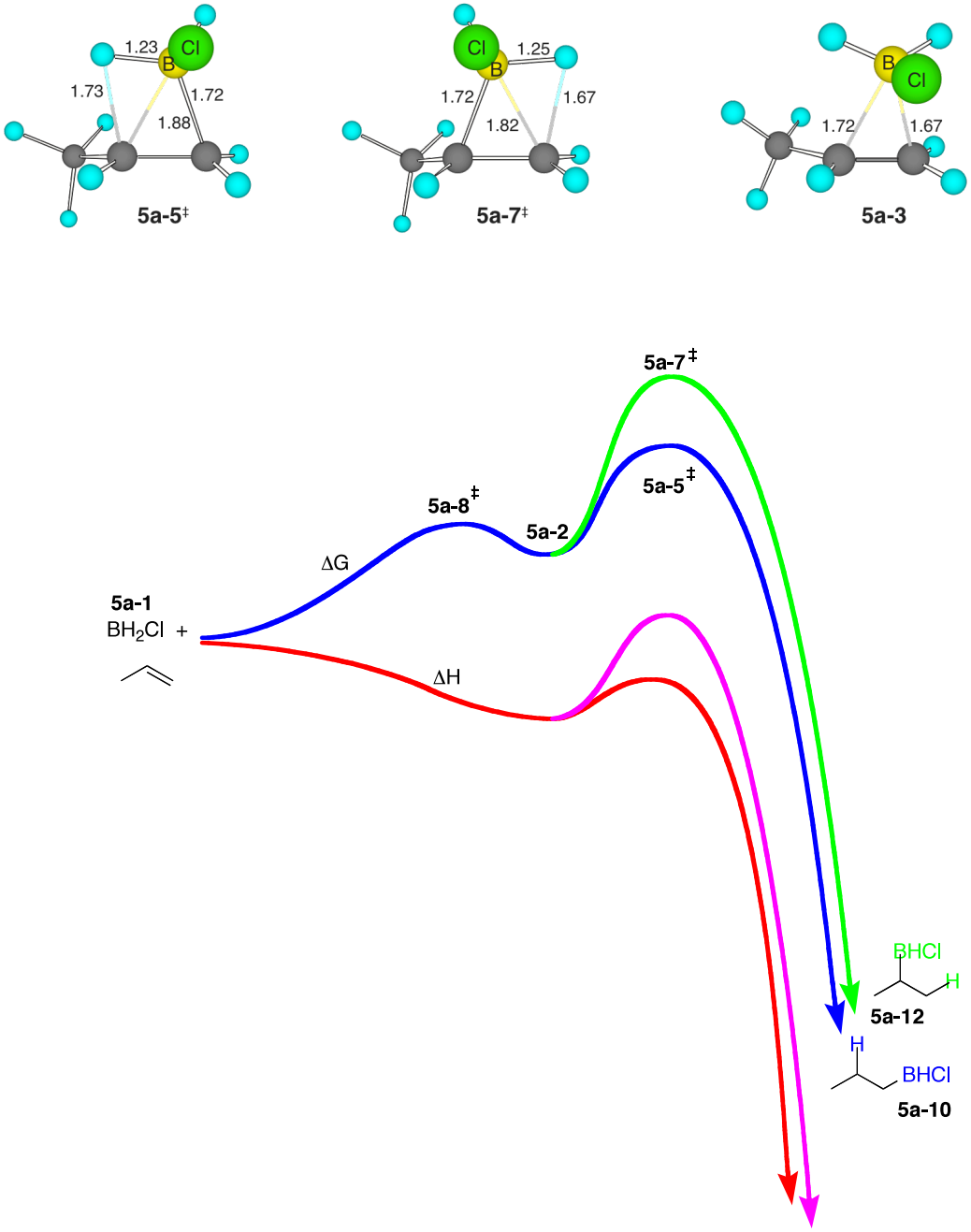


Figure 5.2. G3B3, ΔH and ΔG reaction coordinate diagrams for the lowest energy structures located for the hydroboration of propene with BH_2Cl after anharmonic corrections.

The predicted association barriers found in this case are much lower in energy than the barriers for the formation of products. Figure **5.1** is the reaction coordinate diagram depicting the energetics of the lowest energy conformation structures located for the hydroboration of propene with BH_2Cl. Before considering possible reasons that may account for the discrepancy between theory and experimental results, the second-order perturbative anharmonic contributions to the vibrational energies and entropy were calculated. The free energies for all the structures adjusted are contained in Table **5.2**.

The only major correction from this process was for structure **5a-2**, which is lower in energy than the variational transition structures **5a-8**‡ and **5a-9**‡. by ~ 1.0 kcal/mol. This does not leave room for the possibility of excess energy available to form the product faster than at thermal equilibration. For this case, as can be observed in the new reaction coordinate for energies after anharmonic adjustments (Figure **5.2**), the rate-limiting step for the formation of regioisomeric products is the consequent separate transition states. Therefore, this is not a case of a dynamic effect.

It is important to note that ideally if the transition states leading to the two products are the rate-liming step then we should be able to assume the applicability of transition state theory to predict the selectivity. However, as mentioned previously, when the hydroboration was done with monochloroborane coordinated to different compounds such as SMe_2, dioxane and neat solutions, the ratios do not match the predicted ones.

Table 5.2. Enthalpies and free energies of structures located for the hydroboration of propene with BH_2Cl after anharmonic adjustments.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
5a-2	$\Delta G = 4.6$	$\Delta G = 7.0$	$\Delta G = 9.0$
5a-3	$\Delta G = 6.8$	$\Delta G = 9.1$	$\Delta G = 11.1$
5a-4 ‡	$\Delta G^{\ddagger} = 10.4$	$\Delta G^{\ddagger} = 15.2$	$\Delta G^{\ddagger} = 14.2$
5a-5 ‡	$\Delta G^{\ddagger} = 10.2$	$\Delta G^{\ddagger} = 15.3$	$\Delta G^{\ddagger} = 13.7$
5a-6 ‡	$\Delta G^{\ddagger} = 14.2$	$\Delta G^{\ddagger} = 19.2$	$\Delta G^{\ddagger} = 18.5$
5a-7 ‡	$\Delta G^{\ddagger} = 12.8$	$\Delta G^{\ddagger} = 17.6$	$\Delta G^{\ddagger} = 16.6$

We next considered possible reasons for this discrepancy since the likelihood of dynamic trajectories was eliminated. Consideration of other reaction energetics might suggest an explanation for the inability of transition state theory to account for the product ratio. The energetics of a possible equilibrium of $2BH_2Cl \rightleftarrows BH_3 + BHCl_2$ were calculated. The reverse reaction of the equilibrium is preferred. The free energy for the formation of products in the forward reaction according to DFT methods, G3B3, B3LYP/6-31G* and B3LYP/6-31+G** is 2.5, 3.7 and 3.5 kcal/mol respectively. The

enthalpy for the formation of products in the forward reaction according to (method/basis set) G3B3, B3LYP/6-31G* and B3LYP/6-31+G** is 2.0, 3.7 and 3.5 kcal/mol respectively.

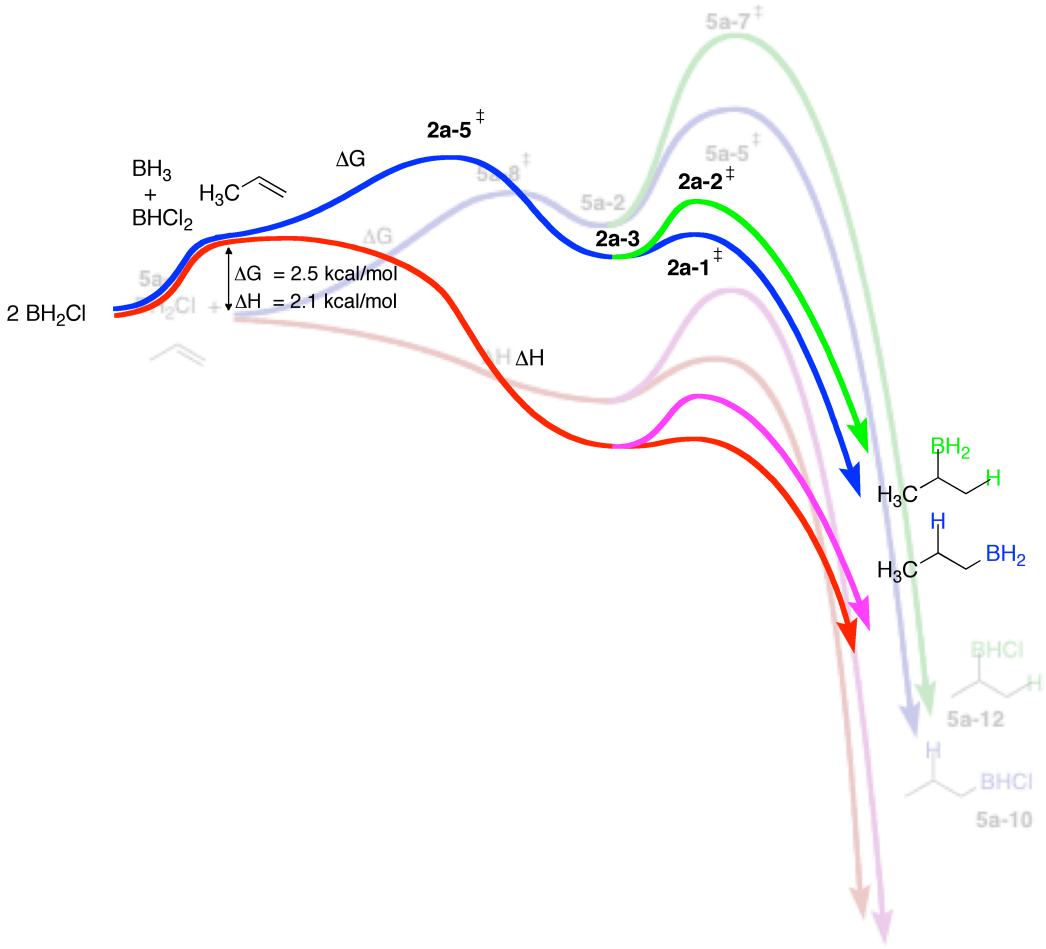


Figure 5.3. G3B3, ΔH and ΔG reaction coordinate diagrams for $2BH_2Cl \rightleftarrows BH_3 + BHCl_2$ follow by the hydroboration of propene with BH_3.

We compared the barriers for the formation of BH_3 along with the energetics of the hydroboration of propene/BH_3 and the barrier for the formation of the anti-Markovnikov product from propene/BH_2Cl. From the G3B3 energies, the barrier for the formation of BH_3 and the barrier hydroboration of propene/BH_3 together required

slightly more energy. In terms of free energy, a first barrier of 2.1 kcal/mol followed by 11 kcal/mol downhill to a second barrier of 0.8 kcal/mol was found for the formation of the anti-Markovnikov product. In terms of enthalpy, the formation of the anti-Markovnikov product from propene/BH_2Cl there would be a barrier of 1.6 kcal/mol, nonetheless, for the formation of the association transition state is only 2.0 kcal/mol downhill. The reaction coordinate of the proposed path is pictured in Figure **5.3**, the shadowed picture behind is the reaction coordinate for the reaction with monochloroborane for comparison with propene/BH_2Cl.

In the case of the Markovnikov product formation the barrier using borane is 3.1 kcal/mol and using monochloroborane is 5.3 kcal/mol, making the total barriers comparable. Now the two paths are not equivalent due to the fact that dynamics plays a role on the selectivity. Once past the first barrier of 2.1 kcal/mol to produce BH_3 the products, formed in the first femtoseconds, will get to product faster than thermal equilibration and no selectivity is expected.

Finally, we can speculate that most of the Markovnikov product observed experimentally might be a consequence of the formation of some BH_3 from $2BH_2Cl \rightleftarrows BH_3 + BHCl_2$. If this is the case, Chapter II described in detail the moderate selectivity of the hydroboration of propene/BH_3 that is expected. Due to the fact that the reverse reaction in the equilibrium is favored, we can expect better selectivity than that of the hydroboration with BH_3 alone.

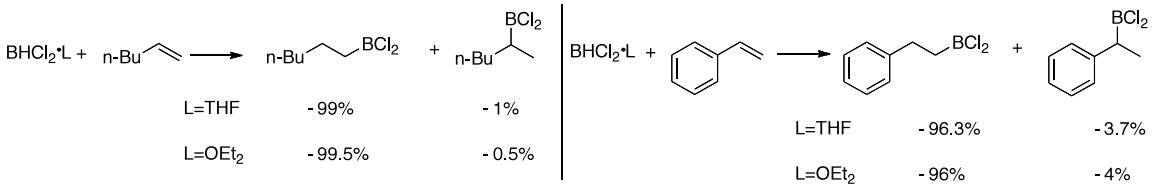
This theory helps explain the modest regioselectivity Brown, Pasto and Zweifel observed for the hydroboration of 1-hexene with monochloroborane in tetrahydrofuran.

The ratios reported were near or identical to the ratios for the hydroboration of 1-hexene with BH_3.

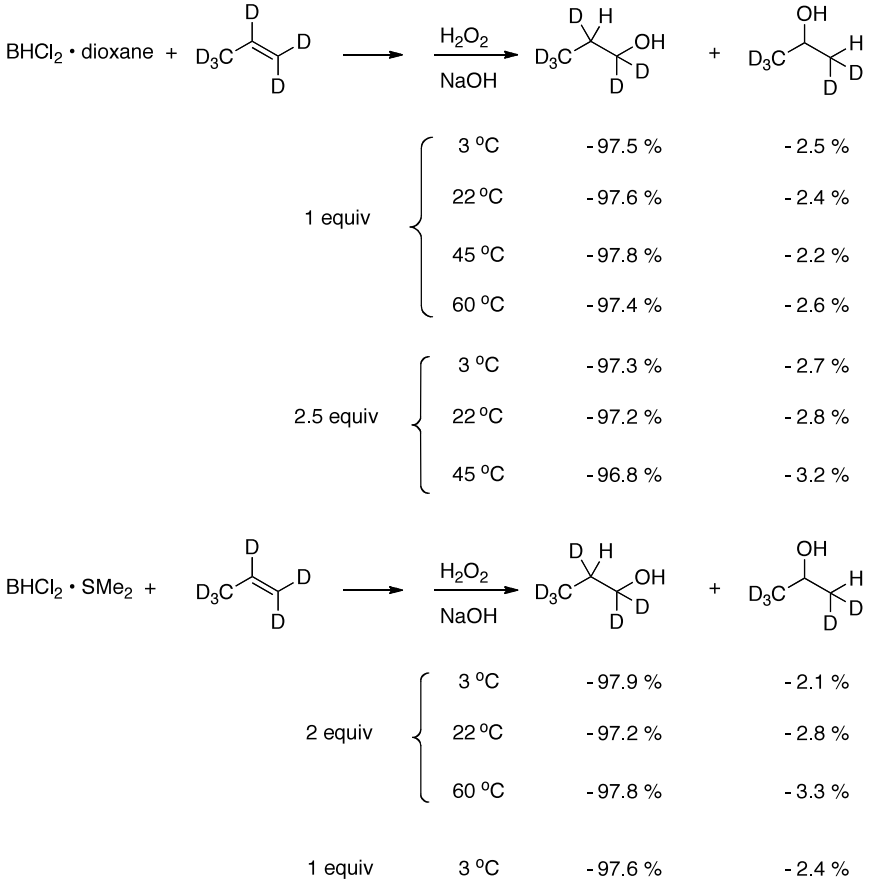
Hydroboration of Alkenes with $BHCl_2$

Dichloroborane has been successfully used for the hydroboration of olefins with high regioselectivity. Relative to borane and monochloroborane, dichloroborane is more acidic in tetrahydrofuran.[29] Dichloroborane has greater acceptor abilities towards the alkene than borane and monochloroborane. This was used to explain why the dichloroborane has a greater ability to form stable π-complexes with the alkenes.[31, 27] On the other hand, this increased stability of complexation causes the reactivity of the hydroboration agent to decrease.[29] Brown has mentioned that in the hydroboration with dichloroborane and ethyl etherate, which is also a very slow reaction when compared to monochloroborane, the reaction rate may be accelerated by adding boron trichloride (a stronger Lewis acid) to the reaction.[37] Kinetic studies of detaching the coordinating agent ($BHCl_2$•SMe_2) suggested a dissociative mechanism. The hydroboration mechanism was determined to be associative, where the first step is the rate-limiting step.[31]

Scheme 5.5



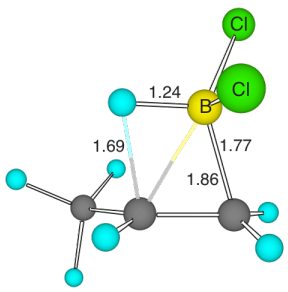
Scheme 5.6



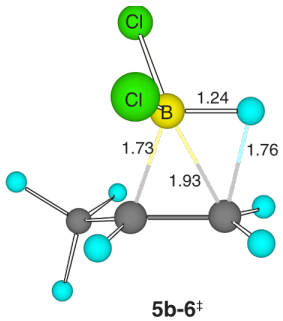
The best selectivity has been observed with dichloroborane as a reagent. The reported explanation is the electronic consideration that favors the transition state leading to the anti-Markovnikov product.[29] The ratio of 1-hexanol to 2-hexanol was 99:1 for the hydroboration of 1-hexene in THF. In addition, the hydroboration of styrene in THF afforded a ratio of 96.3:3.7 of 2-phenylethanol to 1-phenylethanol.[31] Similar ratios have been reported for $BHCl_2$•OEt_2 using pentane as solvent. The ratios are identical to those in the literature for BH_2Cl•OEt_2 with pentane.[34]

Experimentally, we find lower selectivity than previously reported. The reactions, as in the previous case, were directly analyzed by ^{2}H NMR. No purification was required and in cases where layers in the mixture separated, additional water or methanol was added in order to homogenize the solution. In our hands, the selectivity in the hydroboration of propene-d_6 with $BHCl_2$•dioxane and with $BHCl_2$•SMe_2 is analogous to the selectivity obtained in the hydroboration of propene-d_6 with BH_2Cl•dioxane and with BH_2Cl•SMe_2. The experimental ratio in these two cases if assuming the applicability of transition state theory represents a $\Delta\Delta G^{\ddagger}$ of ~2.1 kcal/mol.

Different ratios were obtained for the hydroboration of propene-d_6 when the $BHCl_2$ was generated in situ from trichloroborane and triethylsilane. When the reaction was done in a 1:1 ratio of alkene to borane only one product was detectable by ^{2}H NMR. With an excess of trichloroborane and triethylsilane relative to propene-d_6, 1.3% of the Markovnikov product was detected. Assuming the applicability of transition state theory, the $\Delta\Delta G^{\ddagger}$ for the transition states leading to the two products would be ~2.6 kcal/mol.



5b-5‡



5b-6‡

The experimental selectivity in the hydroboration of simple alkenes with $BHCl_2$ is not in agreement with transition state theory. This was concluded after transition state structures **5b-5**‡ and **5b-6**‡ were located from B3LYP/6-31G* and B3LYP/6-31+G**

calculations for the formation of both regioisomeric products. Table **5.3** summarizes the G3B3, B3LYP/6-31G* and B3LYP/6-31+G** free energies and enthalpies of the structures located. The experimental ratio expected from transition state theory according to the calculations is 99.9:0.1, suggesting that the only obtainable product is formed from **5b-5**‡.

Scheme 5.7

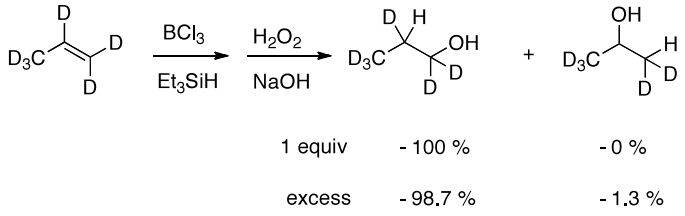


Table 5.3. Enthalpies and free energies of structures located for the hydroboration of propene with $BHCl_2$.

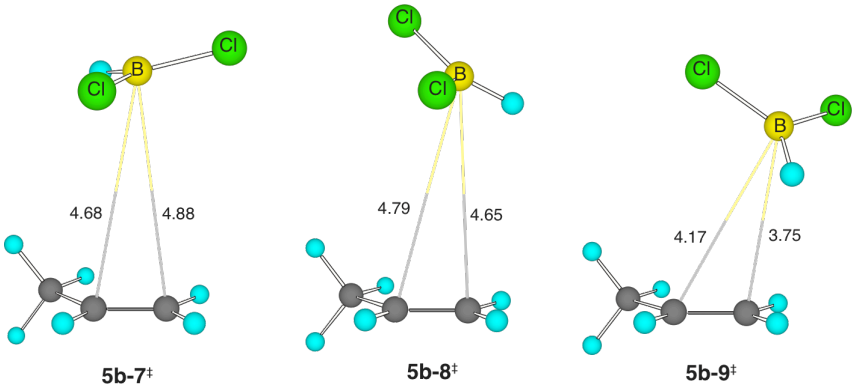
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
5b-1	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0
5b-2	ΔG = 4.5 ΔH = - 2.3	ΔG = 6.9 ΔH = - 1.4	ΔG = 6.0 ΔH = - 0.4

Table 5.3 continued.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
5b-3	$\Delta G = 4.8$ $\Delta H = -2.2$	$\Delta G = 7.1$ $\Delta H = -1.3$	$\Delta G = 6.6$ $\Delta H = -0.5$
5b-4	$\Delta G = 6.3$ $\Delta H = -2.5$	$\Delta G = 8.5$ $\Delta H = -1.2$	$\Delta G = 6.0$ $\Delta H = -0.3$
5b-5‡	$\Delta G^{\ddagger} = 21.0$ $\Delta H^{\ddagger} = 7.8$	$\Delta G^{\ddagger} = 24.2$ $\Delta H^{\ddagger} = 9.9$	$\Delta G^{\ddagger} = 25.6$ $\Delta H^{\ddagger} = 11.4$
5b-6‡	$\Delta G^{\ddagger} = 24.9$ $\Delta H^{\ddagger} = 11.6$	$\Delta G^{\ddagger} = 28.9$ $\Delta H^{\ddagger} = 14.3$	$\Delta G^{\ddagger} = 30.4$ $\Delta H^{\ddagger} = 10.8$
5b-7‡	$\Delta G^{\ddagger} = 6.1$ $\Delta H^{\ddagger} = -0.8$	$\Delta G^{\ddagger} = 6.8$ $\Delta H^{\ddagger} = -0.2$	$\Delta G^{\ddagger} = 9.2$ $\Delta H^{\ddagger} = -0.2$
5b-8‡	$\Delta G^{\ddagger} = 5.7$ $\Delta H^{\ddagger} = -1.4$	$\Delta G^{\ddagger} = 7.1$ $\Delta H^{\ddagger} = -0.8$	$\Delta G^{\ddagger} = 7.8$ $\Delta H^{\ddagger} = -0.3$
5b-9‡	$\Delta G^{\ddagger} = 7.6$ $\Delta H^{\ddagger} = -1.9$	$\Delta G^{\ddagger} = 8.9$ $\Delta H^{\ddagger} = -0.7$	$\Delta G^{\ddagger} = 9.3$ $\Delta H^{\ddagger} = -0.3$
5b-10	$\Delta G = -19.4$ $\Delta H = -30.9$	$\Delta G = -14.8$ $\Delta H = -29.8$	$\Delta G = -12.9$ $\Delta H = -27.7$
5b-11	$\Delta G = -20.0$ $\Delta H = -31.4$	$\Delta G = -16.7$ $\Delta H = -31.4$	$\Delta G = -14.9$ $\Delta H = -29.6$

Furthermore, the discrepancies in the selectivity here cannot be explained by consideration of dynamic trajectories either. The barriers for the formation of products

are too large for the products to form faster than thermal equilibration with solvent. As in the other hydroboration cases, an association barrier was found. The barrier corresponds to the free energy maximum along the steepest-descent path obtained using a modified version of PROGDYN.[84] The structures located, **5b-7**‡, **5b-8**‡, **5b-9**‡, correspond to $BHCl_2$ approaching the propene or the position of the hydrogen atom in the structure. These were the lowest-energy structures found in a re-optimization of π-complexes. Structures **5b-2**, **5b-3** and **5b-4**, were located for the various positions of $BHCl_2$ and propene centroids separated by 5 Å. The G3B3 free energy barriers, from separate starting material to π-complexes structures (**5b-2**, **5b-3** and **5b-4)** are only 6.1, 5.7 and 7.6 kcal/mol for **5b-7**‡, **5b-8**‡and **5b-9**‡, respectively. As we mentioned, this association barrier is significantly lower in energy than the barriers associated with the formation of product.



Corrections for second-order perturbative anharmonic contributions to the vibrational energies and entropy were calculated[85] for the main structures located for propene-d_6/$BHCl_2$ for more accurate predictions (Table **5.4**). Yet, we find no significant

changes in the energetics. The reaction coordinate diagram in Figure **5.4** better represents the energetics described for this system.

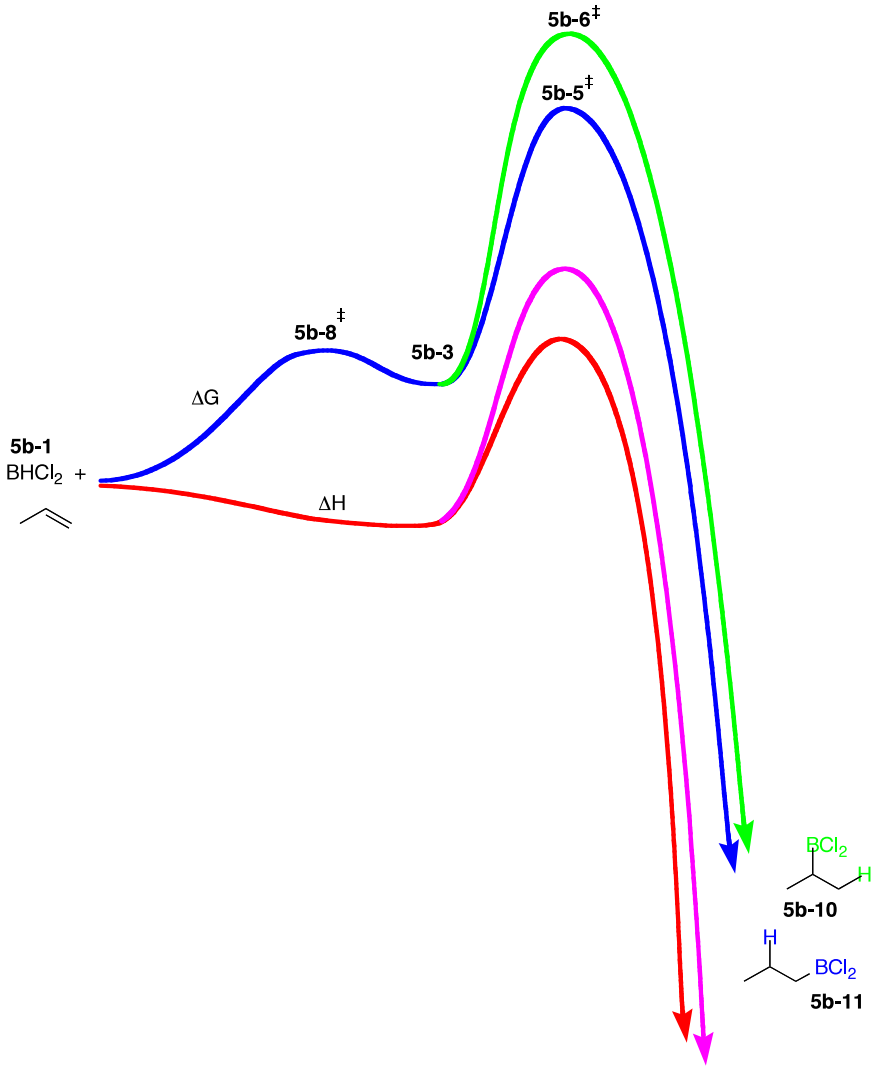


Figure 5.4. G3B3 ΔH and ΔG reaction coordinate diagrams for lowest energy structures located for the hydroboration of propene with $BHCl_2$ after anharmonic corrections.

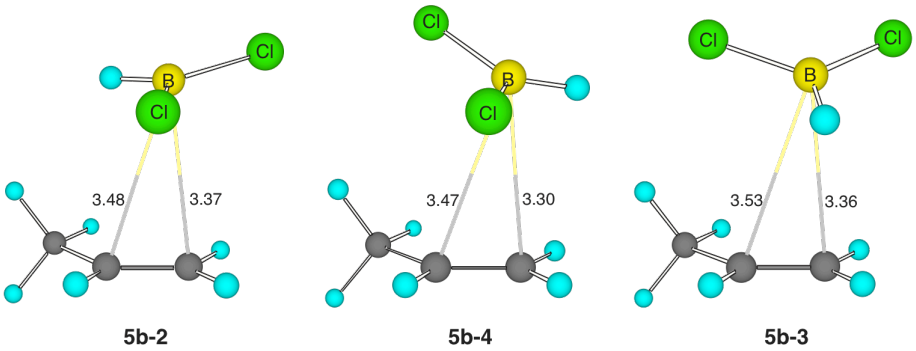


Table 5.4. Enthalpies and free energies of structures located for the hydroboration of propene with $BHCl_2$ after anharmonic adjustments.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
5b-2	ΔG = 4.9	ΔG = 7.2	ΔG = 6.4
5b-3	ΔG = 5.5	ΔG = 7.8	ΔG = 7.3
5b-4	ΔG = 5.4	ΔG = 7.5	ΔG = 6.4
5b-5‡	$\Delta G^{‡}$ = 20.9	$\Delta G^{‡}$ = 24.1	$\Delta G^{‡}$ = 25.5
5b-6‡	$\Delta G^{‡}$ = 24.3	$\Delta G^{‡}$ = 28.3	$\Delta G^{‡}$ = 29.8

Neither of the theories so far were able to explain the moderate experimental selectivity observed here. Virtually no minor product is expected according to the

theoretical results. As was the case for the hydroborating agent BH_2Cl, a small entropic association barrier was located and the energy was considered to be too close to that of the π-complex. Thus, no excess energy was available to facilitate the formation of the Markovnikov product. In other words, it is difficult to overcome a huge enthalpic barrier of formation of ~13.7-15 kcal/mol.

Consideration of an equilibrium $2BHCl_2 \rightleftarrows BCl_3 + BH_2Cl$ presents a possible explanation for the experimental regioselectivity. This process favors the reverse reaction. The barrier for the forward reaction was predicted with DFT methods; G3B3, B3LYP/6-31G* and B3LYP/6-31+G**, the ΔH is 3.5, 5.1 and 5.2 kcal/mol respectively. The free energy is 4.2, 5.4, and 5.5 kcal/mol accordingly.

Referring to the G3B3 enthalpies, the barrier for the formation of BCl_3 and BH_2Cl from $BHCl_2$ is 11.5 kcal/mol lower than that of the formation of the Markovnikov product. However, another barrier for the formation of the Markovnikov product originating from BH_2Cl was also calculated to be 5.3 kcal/mol. Together these barriers require less energy than the barrier for formation for Markovnikov product from dichloroborane. The contrasted relative barriers were put side by side in the reaction coordinate diagram depicted in Figure **5.5**. The reaction coordinate with the implicated barrier for the conversion of $BHCl_2$ to BCl_3 and BH_2Cl, followed by the energetics calculated for the BH_2Cl system. For comparison the energetics for the $BHCl_2$ system, are faded.

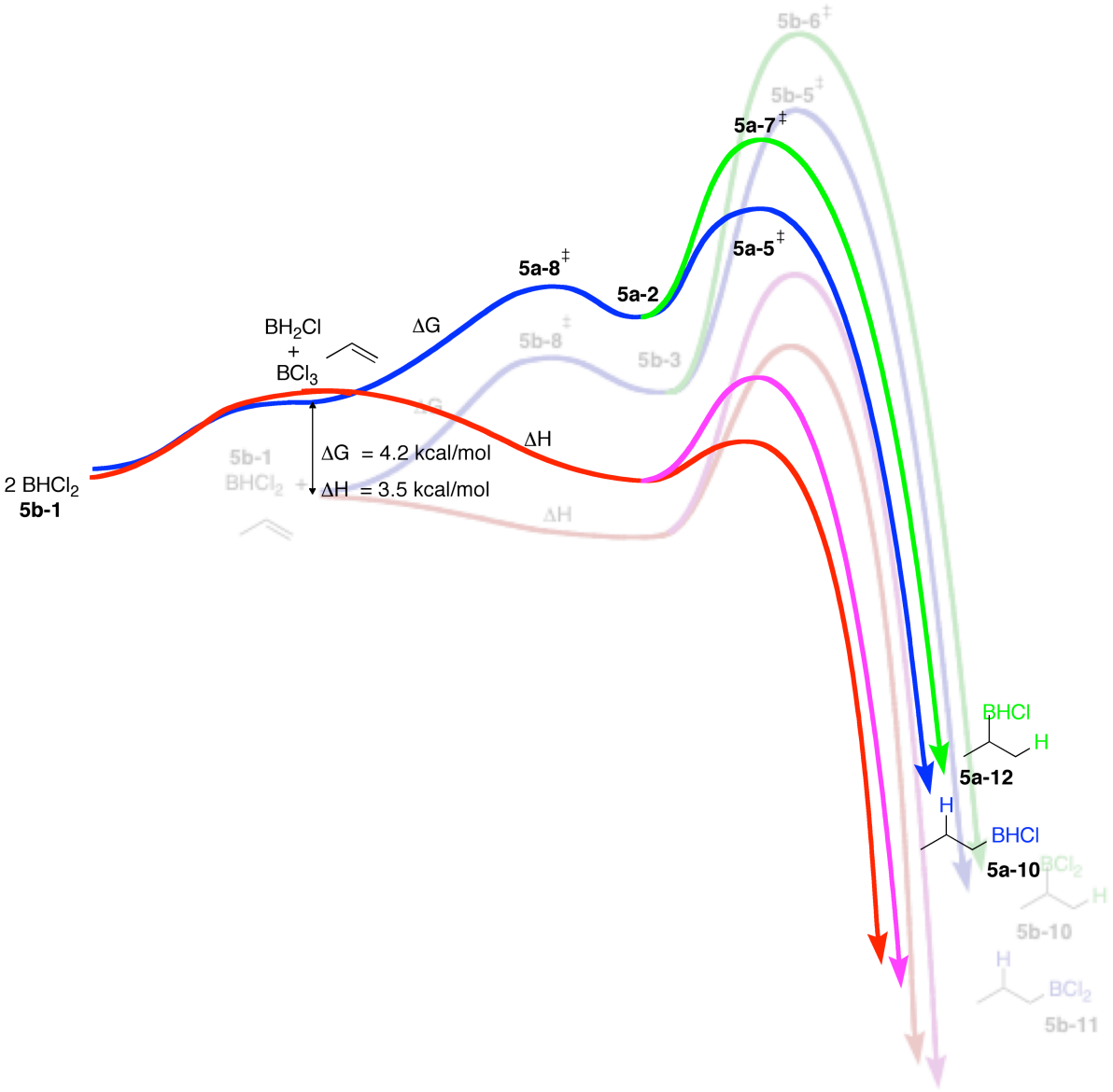


Figure 5.5. G3B3 ΔH and ΔG reaction coordinate diagrams for $2BHCl_2 \rightleftarrows BCl_3 + BH_2Cl$ follow by the hydroboration of propene with BH_2Cl.

Ultimately, we can contemplate that the experimentally observed Markovnikov product may be a consequence of the formation of some BH_2Cl from $2BHCl_2 \rightleftarrows BCl_3 + BH_2Cl$. If this is the case, we can refer to the case above for the explanation of the

experimental regioselectivity. As a consequence we should also consider the theories for the hydroboration of propene/BH_3 to take part on this assumption.

This hypothesis might also help explain the experimental results that were previously reported. Zweifel found the ratio of 1-hexanol to 2-hexanol was 99:1 for the hydroboration of 1-hexene in THF, which is the selectivity expected for the hydroboration of simple alkenes with monochloroborane.[34] Moreover, Brown reported that the hydroboration of styrene with dichoroborane in THF afforded a ratio of 96.3:3.7 of 2-phenylethanol to 1-phenylethanol, which is more moderate.[31] Even when we did not compare styrene theoretically for additional hydroborating agents, Brown points that similar ratios were obtained for $BHCl_2$•OEt_2 using pentane as solvent. These ratios were identical to those he detected for BH_2Cl•OEt_2 with pentane.[34]

A more crucial piece of information that fits here is the observation by Brown for $(ClCH_2CH_2)_2O$•$BHCl_2$ in dichloromethane.[35(b)] Using this reagent with a variety of olefins he was able to measure the amount of BCl_3 generated by ^{11}B NMR. At room temperature, an 8% of BCl_3 was generated from the reaction of 1-octene with dichloroborane. The amount of R_2BCl generated was 2%, relative to the amount of $RBCl_2$. For the reaction with other alkenes like cyclohexene, 50% of BCl_3 and 28% of R_2BCl were detected.

CHAPTER VI

DYNAMICS AND SELECTIVITY IN THE HYDROBORATION OF CHLORO- AND ETHER- SUBSTITUTED ALKENES

Introduction

Our previous chapters studied the dynamic effect with various alkene structures. In the mid 1960's Brown and Pasto carried out systematic studies on the influence of functional groups provided on the placement of boron in the hydroboration of alkenes. In particular, vinyl halide and vinyl ethoxy substituted derivatives. We have recently proposed that transition state theory does not provide an accurate description of the reaction mechanism, but dynamic effects play an active role in the hydroboration of BH_3 with various alkenes. Exploring the dynamic effect idea to vinyl derivatives with halogen and ethoxy groups seems intriguing. To explore the impact of dynamics on alkenes with electronegative substituents we selected a representative group of vinyl derivatives with halide or ethoxy substituents.

The regioselectivity of hydroboration of vinyl derivatives with various substituents has exhibited some interesting results. Early studies of the hydroboration of vinyl chloride and ethyl vinyl ether afforded products with the boron on the β-position. (β-chlorethylboron and tris(ethoxyethyl)borane).[96] Stone and co-workers reacted diborane with a series of flouroethylene derivatives to produce ethylboron fluorides.[97] Brown observed that substituents on styrene influenced the direction of hydroboration and this effect was related to the σ^+ values of the substituents.[18,98] Based on these reported studies, Brown postulated that the substituents, including halides and ethoxy

functional groups, should be capable of producing α-haloorganoboranes, which could then be used for carbene formation.[99]

The idea that substituent groups may have such an effect was seen in the hydroboration of allyl chloride where 40% of the boron attached to the Markovnikov position as compared to only 6% compared to the parent hydrocarbon.[22,100] In the case of 4-pentyl tosylate the hydroboration reaction gave a 45% product composition on the secondary carbon.[22] In the same study, the hydroboration of 1-chloro-3-butene afforded a product ratio of 82:18 of primary to secondary isomers in contrast to the 94:6 ratio observed for simple alkenes.

In addition, the reaction of diborane in THF at 0 °C with allyl acetate, benzoate, borate, alcohol, phenyl ether, ethyl ether, thioether, afforded 19-35% of the Markovnikov product. Pasto found that in the hydroboration of vinyl halides the boron bonded to the carbon bearing the halogen and α-haloorganoboranes formed carbenes by undergoing rearrangements that replace the halogen with hydrogen instead of by α-elimination.[21]

Pasto also observed that the formation of α-substituted organoboranes occurs when the functional group contains ethoxy,[101] and phenylmercapto, or benzylmercapto groups.[102] Brown investigated the hydroboration of vinyl derivatives and found that the reactions of isobutenyl chloride and isobutenyl acetate proceed slowly and placed boron almost exclusively in the α-position.[24] In the case of hydroboration of the ethoxy derivative, a rapid reaction occurs and boron added to the β-position.[24]

The reactivity and selectivity of the hydroboration of vinyl derivatives containing halide and ethoxy groups has generally been explained using electronics as the predominant factor. However, the selectivity in hydroboration has been considered as the results of the two different transition state barriers that lead to alternative products. As state, in a previous chapter, this has been applied without considering the fact that an exothermic association process with a free energy barrier might be involved and this association free energy barrier could be the rate-limiting step. The combination of the rate limiting association and the potential role of dynamic effects provides a new mechanistic interpretation of experimental observations of experimental reactivities and selectivities with alkenes containing highly electronegative substituents.

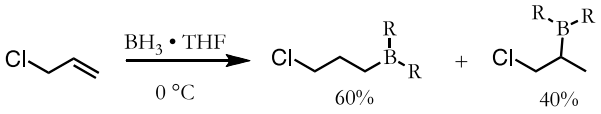
We want to determine if there is a discrepancy between the observed experimental selectivity and that predicted by transition state theory for the BH_3 hydroboration of vinyl derivatives with highly electronegative substituents. If this is the case, we will establish if dynamic effects are involved by considering the energetics for the reaction.

Dynamics and Selectivity in the Hydroboration of Allylchloride with BH_3

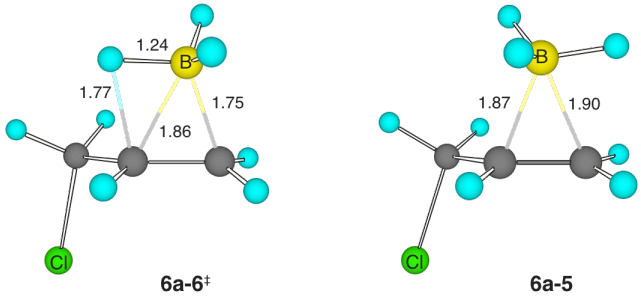
An important observation in the hydroboration of allyl chloride with BH_3 is the lower regioselectivity when compared to simple alkenes. Brown reported, what he called the powerful directive effect of chlorine as a close neighbor in hydroboration of double bonds, to cause a striking 40% Markovnikov product.[22] For the hydroboration of allyl chloride with disiamylborane as a hydroboration agent, approximately 3% Markovnikov product and 82% anti-Markovnikov product was detected.[29] Is necessary

to point out the complication of the experimental analysis in place of the Markovnikov product, the elimination of the neighboring boron and chlorine atoms. This elimination affords, in the case of allyl chloride, propene, which may perhaps be hydroborated further.[22] The complication of the experimental analysis of the anti-Markovnikov product is the cyclization of the γ-chloropropylborane to produce cyclopropane. An advantage to this cyclization is that it appears to be quantitative.[103]

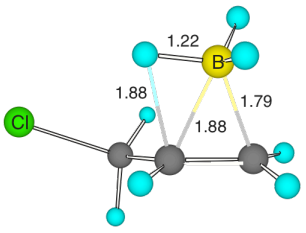
Scheme 6.1



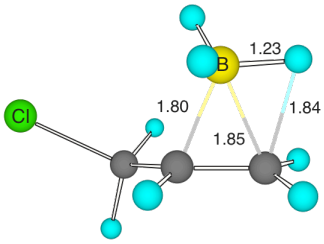
Explanations to the findings in terms of reactivity and regioselectivity of this case were again sterics as the predominant effect. Brown also alluded to the electronic interactions, like induction and hyperconjugation, which are electron withdrawing effect reducing the rate. Selectivity reduction was attribute to conjugation returning electron density to the β position to become appealing for hydroboration.



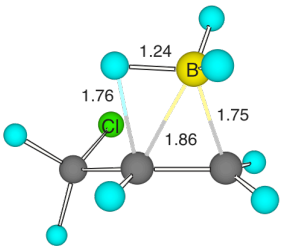
If we assume the applicability of the transition state theory, the $\Delta\Delta G^{\ddagger}$ for the transition states leading to product and the experimental selectivity should show agreement. The $\Delta\Delta G^{\ddagger}$ according to the experimental regioselectivity found by Brown for the hydroboration of allylchloride with BH_3 in tetrahydrofuran is 0.2 kcal/mol. A computational approach was taken in an effort to predict the $\Delta\Delta G^{\ddagger}$ and the transition structures **6a-6**‡**, 6a-7**‡ and **6a-8**‡ for the formation of the anti-Markovnikov regioisomeric product were located using B3LYP/6-31G* and B3LYP/6-31+G** calculations (Table **6.1**). For the formation of the Markovnikov regioisomeric product structures **6a-9** and **6a-10** were located with the same method/basis sets. The calculations predict an energetic preference for the anti-Markovnikov product that exceeds that implied by the experimental selectivity. This is determined form allowing for contribution from each transition states, according to the calculated free energy. The experiment is significantly less selective than the expected 88:12 predicted from calculations. As a consequence, we come to the conclusion that transition state theory does not provide an explanation for the regioselectivity observed.



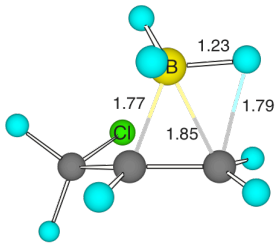
6a-8‡



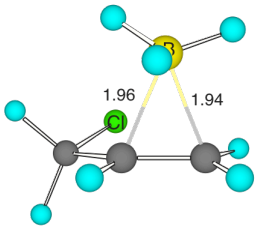
6a-10‡



6a-7‡



6a-9‡



6a-4

Table 6.1. Enthalpies and free energies of structures located for the hydroboration of allylchloride with BH_3.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6a-1	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0
6a-2	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0
6a-3	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0
6a-4	ΔG = 1.4 ΔH = - 8.9	ΔG = 4.6 ΔH = - 8.2	ΔG = 6.2 ΔH = - 6.6
6a-5	ΔG = 0.2 ΔH = - 9.9	ΔG = 2.6 ΔH = - 10.1	ΔG = 4.2 ΔH = - 8.5
6a-6 ‡	$\Delta G^{\ddagger}$ = 0.8 $\Delta H^{\ddagger}$ = - 10.5	$\Delta G^{\ddagger}$ = 5.0 $\Delta H^{\ddagger}$ = - 8.6	$\Delta G^{\ddagger}$ = 4.7 $\Delta H^{\ddagger}$ = - 8.4
6a-7 ‡	$\Delta G^{\ddagger}$ = 3.1 $\Delta H^{\ddagger}$ = - 8.6	$\Delta G^{\ddagger}$ = 8.2 $\Delta H^{\ddagger}$ = - 5.7	$\Delta G^{\ddagger}$ = 7.5 $\Delta H^{\ddagger}$ = - 5.8
6a-8 ‡	$\Delta G^{\ddagger}$ = 4.1 $\Delta H^{\ddagger}$ = - 7.5	$\Delta G^{\ddagger}$ = 11.0 $\Delta H^{\ddagger}$ = - 2.9	$\Delta G^{\ddagger}$ = 7.9 $\Delta H^{\ddagger}$ = 3.7

Table 6.1 continued.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6a-9‡	$\Delta G^{\ddagger} = 2.4$ $\Delta H^{\ddagger} = -8.8$	$\Delta G^{\ddagger} = 7.5$ $\Delta H^{\ddagger} = -6.6$	$\Delta G^{\ddagger} = 7.2$ $\Delta H^{\ddagger} = -6.2$
6a-10‡	$\Delta G^{\ddagger} = 2.4$ $\Delta H^{\ddagger} = -8.5$	$\Delta G^{\ddagger} = 8.5$ $\Delta H^{\ddagger} = -5.4$	$\Delta G^{\ddagger} = 6.7$ $\Delta H^{\ddagger} = -6.4$
6a-11‡	$\Delta G^{\ddagger} = 5.7$ $\Delta H^{\ddagger} = -1.2$	$\Delta G^{\ddagger} = 6.5$ $\Delta H^{\ddagger} = -0.7$	$\Delta G^{\ddagger} = 6.2$ $\Delta H^{\ddagger} = -0.4$
6a-12‡	$\Delta G^{\ddagger} = 5.9$ $\Delta H^{\ddagger} = -0.9$	$\Delta G^{\ddagger} = 7.3$ $\Delta H^{\ddagger} = 0.5$	$\Delta G^{\ddagger} = 6.7$ $\Delta H^{\ddagger} = 0.8$
6a-13‡	$\Delta G^{\ddagger} = 5.1$ $\Delta H^{\ddagger} = -2.0$	$\Delta G^{\ddagger} = 6.1$ $\Delta H^{\ddagger} = -1.2$	$\Delta G^{\ddagger} = 5.9$ $\Delta H^{\ddagger} = -0.6$

After allowing for the second-order perturbative anharmonic contributions (Table **6.2**), the regioselectivity is higher. This was determined from allowing for the contribution from each transition states for the different conformations located, according to the free energy calculated. The computed ratio is now 92:8 for anti-Markovnikov to Markovnikov product, which is an even higher regioselectivity than that observed experimentally.

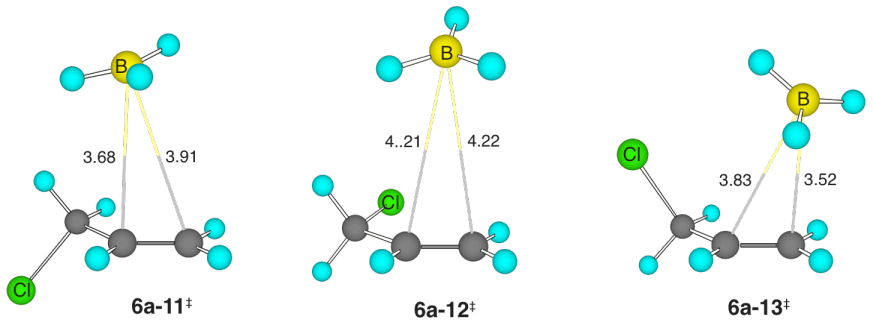
Table 6.2. Enthalpies and free energies of product structures from the hydroboration of allylchloride with BH_3.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6a-14	ΔG = - 21.3 ΔH = - 31.0	ΔG = - 20.4 ΔH = - 33.6	ΔG = - 19.3 ΔH = - 32.0
6a-15	ΔG = - 21.3 ΔH = - 31.5	ΔG = - 20.0 ΔH = - 33.8	ΔG = - 18.1 ΔH = - 31.6
6a-16	ΔG = - 20.7 ΔH = - 31.1	ΔG = - 18.2 ΔH = - 32.1	ΔG = - 16.5 ΔH = - 30.4
6a-17	ΔG = - 20.4 ΔH = - 30.6	ΔG = - 18.2 ΔH = - 32.1	ΔG = - 16.4 ΔH = - 30.2
6a-18	ΔG = - 20.4 ΔH = - 30.6	ΔG = - 14.2 ΔH = - 28.8	ΔG = - 16.7 ΔH = - 30.5

To deduce whether or not the experimental regioselectivity was a result of dynamics, since the applicability of transition state theory clearly fails, we located the variational transition state. The entropic barriers for the association of the BH_3 with different conformations of allylchloride were located (**6a-11**‡, **6a-12**‡ and **6a-13**‡). In terms of free energy the barriers were ~ 2.5-4.0 kcal/mol higher than the barrier for the formation of the Markovnikov product. In other words, the variational transition state provides excess energy for the formation of product for the BH_3/allylchloride reaction.

Table 6.3. Enthalpies and free energies of structures located for the hydroboration of allylchloride with BH_3 after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6a-2	ΔG = 0.1 ΔH = 0.2	ΔG = 0.2 ΔH = 0.2	ΔG = 0.2 ΔH = 0.2
6a-3	ΔG = 0.1 ΔH = 0.1	ΔG = 0.1 ΔH = 0.1	ΔG = 0.1 ΔH = 0.1
6a-4	ΔG = 1.6 ΔH = - 9.0	ΔG = 4.8 ΔH = - 8.3	ΔG = 6.4 ΔH = - 6.7
6a-5	ΔG = - 1.9 ΔH = - 9.7	ΔG = 0.5 ΔH = - 9.9	ΔG = 2.1 ΔH = - 8.3
6a-6‡	$\Delta G^{\ddagger}$ = 0.4 $\Delta H^{\ddagger}$ = - 10.8	$\Delta G^{\ddagger}$ = 4.6 $\Delta H^{\ddagger}$ = - 8.9	$\Delta G^{\ddagger}$ = 4.3 $\Delta H^{\ddagger}$ = - 8.7
6a-7‡	$\Delta G^{\ddagger}$ = 2.5 $\Delta H^{\ddagger}$ = - 8.8	$\Delta G^{\ddagger}$ = 7.7 $\Delta H^{\ddagger}$ = - 5.9	$\Delta G^{\ddagger}$ = 7.0 $\Delta H^{\ddagger}$ = - 6.0
6a-8‡	$\Delta G^{\ddagger}$ = 3.3 $\Delta H^{\ddagger}$ = - 7.5	$\Delta G^{\ddagger}$ = 10.2 $\Delta H^{\ddagger}$ = - 2.9	$\Delta G^{\ddagger}$ = 7.1 $\Delta H^{\ddagger}$ = 3.7
6a-9‡	$\Delta G^{\ddagger}$ = 2.0 $\Delta H^{\ddagger}$ = - 9.1	$\Delta G^{\ddagger}$ = 7.2 $\Delta H^{\ddagger}$ = - 6.9	$\Delta G^{\ddagger}$ = 6.9 $\Delta H^{\ddagger}$ = - 6.5
6a-10‡	$\Delta G^{\ddagger}$ = 2.6 $\Delta H^{\ddagger}$ = - 8.7	$\Delta G^{\ddagger}$ = 8.6 $\Delta H^{\ddagger}$ = - 5.6	$\Delta G^{\ddagger}$ = 6.8 $\Delta H^{\ddagger}$ = - 6.6



As depicted in Figure **6.1**, the formation of the various complexes, found for all corresponding conformations of allylchloride, this is enthalpically barrierless. Excess energy may be available from the formation of the complex and it may pass to product faster than thermal equilibration with solvent can occur.

In summary, the current understanding of regioselectivity in the BH_3/allylchloride reaction assumes the applicability of the transition state theory model of reactivity. It is found here that transition state theory cannot explain the experimental ratio of products for the hydroboration of allylchloride with BH_3. High-level calculations predict too large of an energy difference between competitive transition structures to account for the observed product ratio. Consideration of perturbative anharmonic contributions, Table **6.3**, does not resolve the discrepancy, contrary it predicts a higher selectivity between competitive transition structures. Consideration of the reaction energetics suggests an explanation for the inability of transition state theory to account for the product ratio. This is true because considerable excess energy is thus available from the formation of π-complexes, and the barriers for formation of products from structure, **6a-5** are quite small.

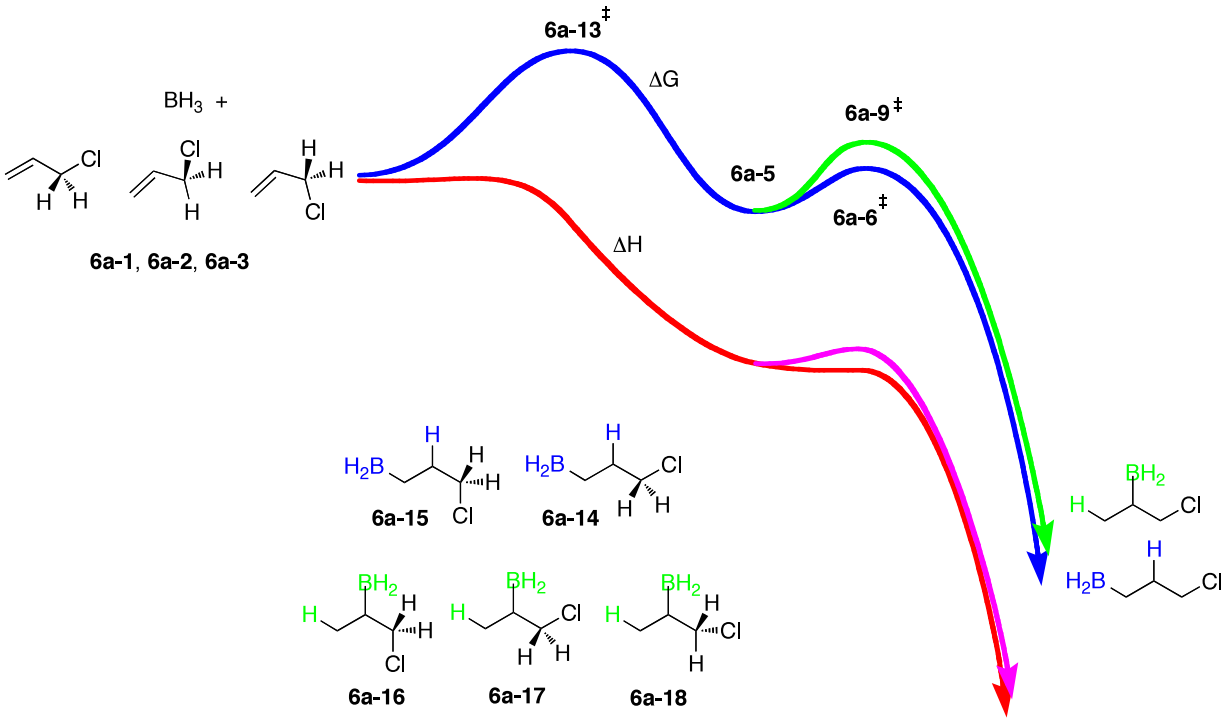


Figure 6.1. Free energy and enthalpy reaction coordinate diagram for the hydroboration of allylchloride with BH_3, representing the lowest energy conformation for each point.

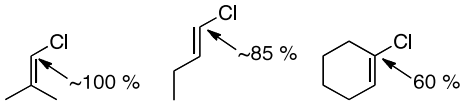
Calculated Pathway for the Hydroboration of Chlorocyclohexene with BH_3

The hydroboration of vinyl chloro-olefins reported by Brown showed a preference to place the boron on the α-carbon.[24] There are some synthetic complications when the boron adds to the β-carbon because of the possible elimination of the boron-chloro and re-hydroboration can occurs with the resulting alkene. For this observation it has been proposed by Pasto, a "transfer reaction".[21] The "transfer reaction" was explained as an intramolecular exchange of hydride and chlorine.

Brown analyzed various vanylchloride for patterns that would aid in making predictions of unexplored systems. For the hydroboration of variousvinyl chlorides and

borane in tetrahydrofuran, the favored product was the one formed by addition of the boron on the α-carbon as shown in Scheme **6.2**.

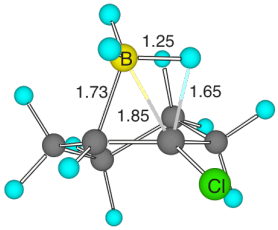
Scheme 6.2



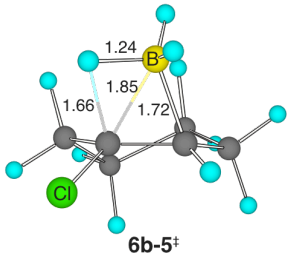
We were interested in exploring possible explanations for the experimental selectivity observed for 1-chlorocyclohexene. Brown described an attractive influence of chlorine for the boron to explain the experimental inclination of the vinyl chlorides to afford the boron on the α-carbon. In other words, the boron attaches to the most substituted carbon if one of the substituents was chlorine, which goes against the alkyl-substituted alkenes tendencies. However, for 1-chlorocyclohexene, this directive effect was not so powerful. The selectivity was only 40:60 anti-Markovnikov to Markovnikov (we will refer to anti-Markovnikov product for the product with boron on the β-carbon, which is the least substituted carbon). Assuming the applicability of transition state theory, the $\Delta\Delta G^{\ddagger}$ for the transition states leading to the two products would be 0.2 kcal/mol strikingly towards the most substituted side of the alkene, opposite to what we had discussed in previous chapters.

Three gas-phase computational approaches were explored in an attempt to predict this $\Delta\Delta G^{\ddagger}$. From G3B3 energies we predicted an energetic preference for both transition states located **6b-4**‡ and **6b-5**‡ leading to the anti-Markovnikov products. The preference for anti-Markovnikov product in this case opposes that implied by the

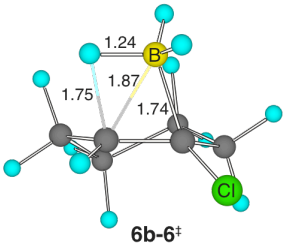
experimental regioselectivity (Tables **6.4** and **6.5**). In other words, the experiment is considerably less selective than the 76:24 expected from the calculations after allowing for the free energies of all possible transition states located.



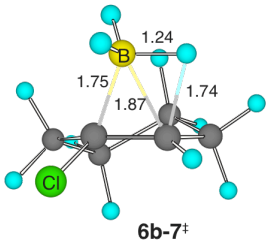
6b-4‡



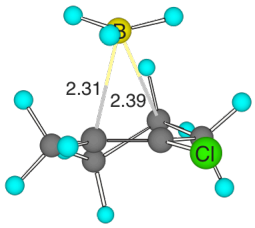
6b-5‡



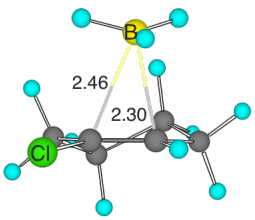
6b-6‡



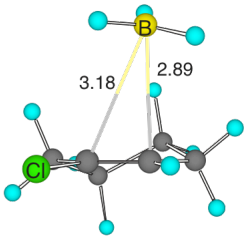
6b-7‡



6b-2



6b-3

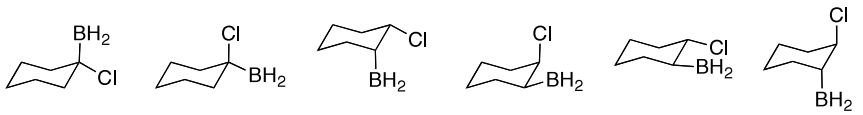


6b-8‡

Table 6.4. Enthalpies and free energies of structures located for the hydroboration of chlorocyclohexene with BH_3.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6b-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
6b-2	$\Delta G = 2.4$ $\Delta H = -7.2$	$\Delta G = 7.4$ $\Delta H = -4.6$	$\Delta G = 8.2$ $\Delta H = -3.6$
6b-3	$\Delta G = 2.6$ $\Delta H = -7.1$	$\Delta G = 7.3$ $\Delta H = -4.6$	$\Delta G = 8.2$ $\Delta H = -3.6$
6b-4‡	$\Delta G^{\ddagger} = 6.8$ $\Delta H^{\ddagger} = -5.1$	$\Delta G^{\ddagger} = 12.8$ $\Delta H^{\ddagger} = -1.0$	$\Delta G^{\ddagger} = 13.2$ $\Delta H^{\ddagger} = -0.6$
6b-5‡	$\Delta G^{\ddagger} = 7.1$ $\Delta H^{\ddagger} = -4.7$	$\Delta G^{\ddagger} = 12.8$ $\Delta H^{\ddagger} = -0.7$	$\Delta G^{\ddagger} = 13.2$ $\Delta H^{\ddagger} = -0.4$
6b-6‡	$\Delta G^{\ddagger} = 7.3$ $\Delta H^{\ddagger} = -4.6$	$\Delta G^{\ddagger} = 12.3$ $\Delta H^{\ddagger} = -1.4$	$\Delta G^{\ddagger} = 12.9$ $\Delta H^{\ddagger} = -0.7$
6b-7‡	$\Delta G^{\ddagger} = 8.4$ $\Delta H^{\ddagger} = -3.4$	$\Delta G^{\ddagger} = 13.3$ $\Delta H^{\ddagger} = -0.4$	$\Delta G^{\ddagger} = 13.9$ $\Delta H^{\ddagger} = 0.3$
6b-8‡	$\Delta G^{\ddagger} = 5.0$ $\Delta H^{\ddagger} = -5.0$	$\Delta G^{\ddagger} = 7.6$ $\Delta H^{\ddagger} = -2.7$	$\Delta G^{\ddagger} = 7.8$ $\Delta H^{\ddagger} = -1.9$

Table 6.5. Enthalpies and free energies of structures located for the products from the hydroboration of chlorocyclohexene with BH_3.



6b-9 **6b-10** **6b-11** **6b-12** **6b-13** **6b-14**

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6b-9	ΔG = - 22.5 ΔH = - 33.8	ΔG = -18.0 ΔH = - 33.2	ΔG = - 16.8 ΔH = - 31.2
6b-10	ΔG = - 22.5 ΔH = - 33.8	ΔG = - 18.0 ΔH = - 33.2	ΔG = - 16.8 ΔH = - 31.9
6b-11	ΔG = - 22.3 ΔH = - 33.5	ΔG = - 17.4 ΔH = - 32.7	ΔG = - 16.2 ΔH = - 31.4
6b-12	ΔG = - 18.3 ΔH = - 29.1	ΔG = - 13.5 ΔH = - 27.9	ΔG = - 12.6 ΔH = - 27.0
6b-13	ΔG = - 18.1 ΔH = - 28.8	ΔG = - 13.9 ΔH = - 28.6	ΔG = - 12.9 ΔH = - 27.6
6b-14	ΔG = - 17.9 ΔH = - 28.9	ΔG = - 13.1 ΔH = - 27.7	ΔG = - 12.3 ΔH = - 26.8

Identical to previous chapters, second-order perturbative anharmonic contributions to the vibrational energies and entropy were calculated[85] for each transition state, complex and starting material, structure and applied as corrections for enthalpies

and free energy. The resulting energetics for this system after these corrections are summarized in Table **6.6**.

Table 6.6. Enthalpies and free energies of structures located for the hydroboration of chlorocyclohexene with BH_3 after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6b-2	ΔG = 0.2 ΔH = - 7.9	ΔG = 5.2 ΔH = - 5.3	ΔG = 6.0 ΔH = - 4.3
6b-3	ΔG = 0.3 ΔH = - 7.0	ΔG = 5.0 ΔH = - 4.6	ΔG = 5.9 ΔH = - 3.6
6b-4‡	$\Delta G^{\ddagger}$ = 6.6 $\Delta H^{\ddagger}$ = - 5.2	$\Delta G^{\ddagger}$ = 12.6 $\Delta H^{\ddagger}$ = - 1.1	$\Delta G^{\ddagger}$ = 13.0 $\Delta H^{\ddagger}$ = - 0.1
6b-5‡	$\Delta G^{\ddagger}$ = 7.3 $\Delta H^{\ddagger}$ = - 4.8	$\Delta G^{\ddagger}$ = 13.0 $\Delta H^{\ddagger}$ = - 0.2	$\Delta G^{\ddagger}$ = 13.4 $\Delta H^{\ddagger}$ = - 0.5
6b-6‡	$\Delta G^{\ddagger}$ = 7.2 $\Delta H^{\ddagger}$ = - 4.7	$\Delta G^{\ddagger}$ = 12.2 $\Delta H^{\ddagger}$ = - 1.5	$\Delta G^{\ddagger}$ = 12.8 $\Delta H^{\ddagger}$ = - 0.8
6b-7‡	$\Delta G^{\ddagger}$ = 7.9 $\Delta H^{\ddagger}$ = - 3.7	$\Delta G^{\ddagger}$ = 12.8 $\Delta H^{\ddagger}$ = - 0.6	$\Delta G^{\ddagger}$ = 13.4 $\Delta H^{\ddagger}$ = 0.1

From corrected G3B3 energies, the prediction was still an energetic preference for both transition states located **6b-4**‡ and **6b-5**‡ leading to the anti-Markovnikov products that contradicts that implied by the experimental selectivity. The computational prediction after the anharmonic adjustments are a ratio of 73:27 expected from the

calculations also allowing for the free energies of all possible transition states located. This implies the inability of transition state theory to account for the experimentally observed product ratio.

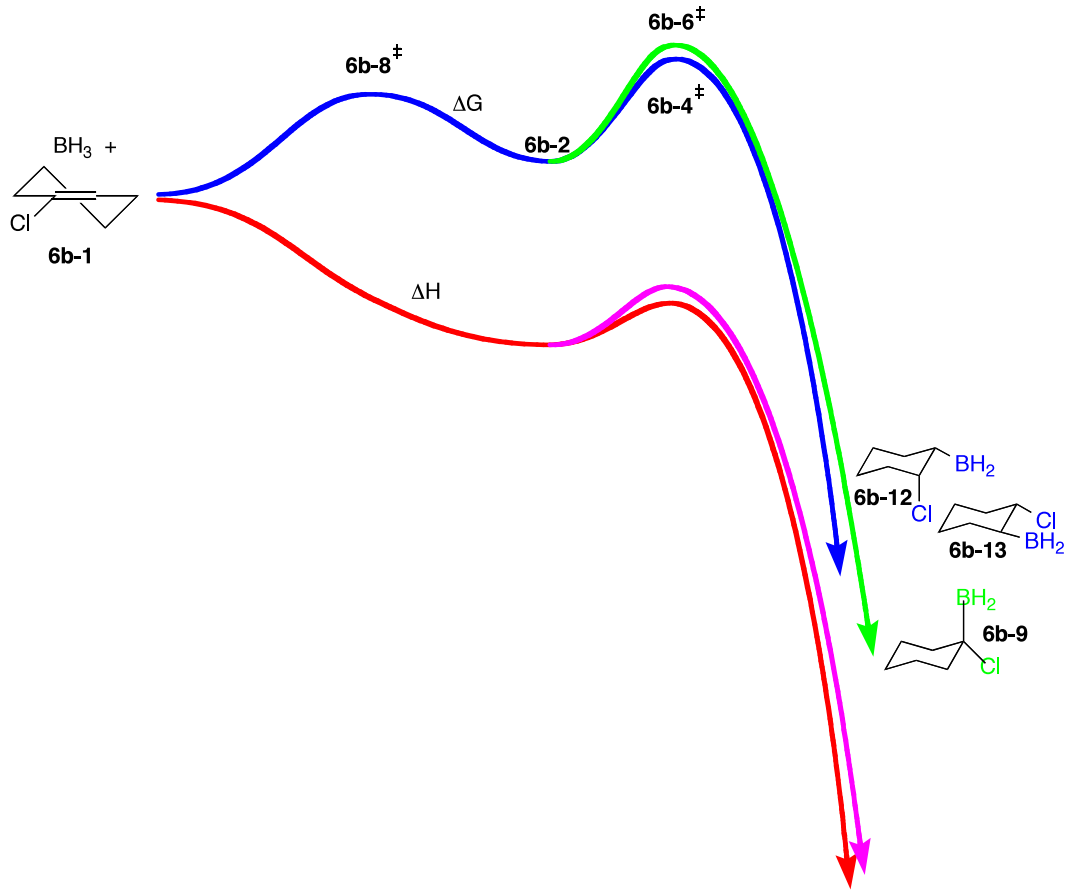


Figure 6.2. Free energy and enthalpy reaction coordinate diagram for the hydroboration of chlorocyclohexene with BH_3, representing the lowest energy conformation for each point.

On the other hand, consideration of the reaction energetics (Figure **6.2**) may suggest an explanation for the shortcomings of transition state theory. As Shown in

Figure **6.2**, the formation of complexes **6b-2** and **6b-3** is enthalpically barrierless and downhill by about 5 kcal/mol from a located entropic association barrier, **6b-8**‡. Excess energy is thus available from formation of the π-complex, however, the barriers for the formation of products are 7.0-7.7 kcal/mol. This piece of evidence makes it difficult to judge whether dynamic effects are play in. Complexes **6b-2** and **6b-3** are enthalpically barrierless and downhill by about 5 kcal/mol trajectories; they may pass to products faster that thermal equilibration with solvent. Nonetheless, the barrier for product formation represents the rate-limiting step in this case and the excess energy may or may not be enough to overcome this 7.0-7.7 kcal/mol barrier faster that thermal equilibration with solvent. Dynamic trajectories may predict the experimental selectivity if the excess energy allows rapid formation of product. This is because the difference in energy predicted between the lowest in energy transition states leading to products is very small, only 0.6 kcal/mol.

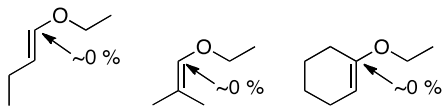
Overall, for this system, it is inconclusive whether it is a case of dynamics or not. More detailed investigation is essential, including consideration of errors.

Dynamics and Selectivity in the Hydroboration of Representative Vinyl Unsaturated Ether with BH_3

As was the case for chlorocyclohexene, Brown analyzed various vinyl ethers for patterns that would allow him to make prediction of unexplored systems.[24] For the hydroboration of the various ethoxy substituted alkenes with borane in tetrahydrofuran

the product was exclusively formed from the addition of the boron on the β-carbon as shown in scheme **6.3**.

Scheme 6.3

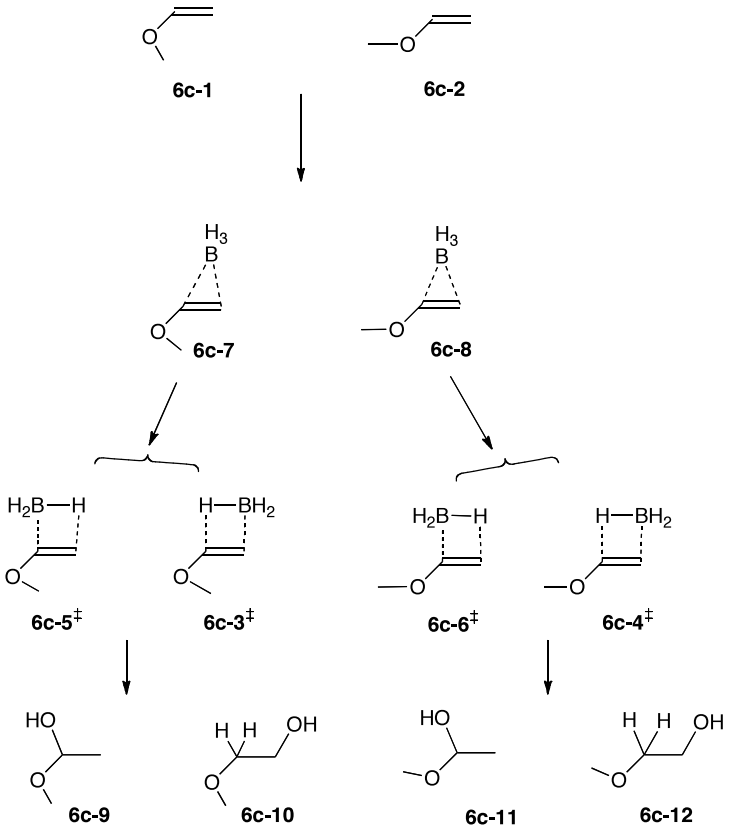


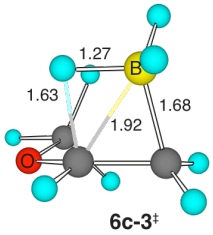
We were interested in explaning the experimental selectivity observed for methyl vinyl ether, isobutenyl methyl and ethyl ethers, as well as the 1-methoxycyclohexene. Brown described the ethoxy substituted as being able to dominate the direction of boron addition to the alkene. He attributed the experimental preference for the boron to add to the most substituted carbon, as was the case in the hydroboration of isobutenyl ethyl ether, to the directive effect of the ethoxy. The inclination for that case was 100 % towards the most substituted alkene.[24] This can be seen as usual for hydroboration as we can compare this case to the hydroboration of 2-methyl-2-butene, where the opposite results were observed, 98% prefer the anti-Markovnikov product (Chapter IV).

To determine the applicability of transition state theory, the energetics for the hydroboration of methyl vinyl ether, isobutenyl methyl and ethyl ethers, as well as the 1-methoxycyclohexene with BH_3 were calculated. The variational transition states for the association of BH_3 with each alkene to afford the π-complex was located by an adaptation of the "nosaddle" procedure of Truhlar and coworkers.[84] The starting point for the location of the variational transition states was the lowest-energy structure found in a scan of positions with BH_3 and each alkene in different conformations, separated by 5 Å.

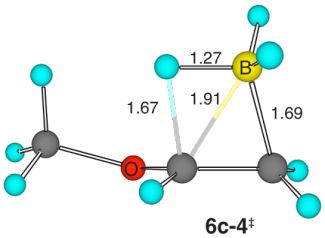
From this structure, a steepest-descent path in mass-weighted coordinates was followed using the program PROGDYN.[84] The free energies and enthalpies determined for each structure of the four systems were summarized in Tables **6.7-6.16** with structure diagrams between them.

Scheme 6.4

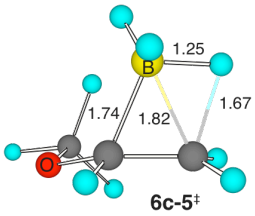




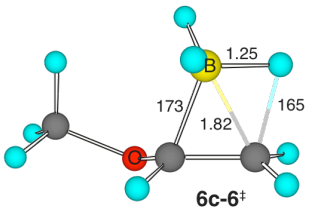
6c-3‡



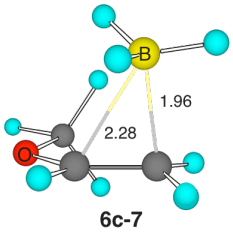
6c-4‡



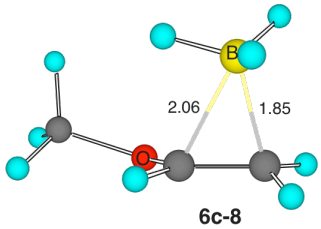
6c-5‡



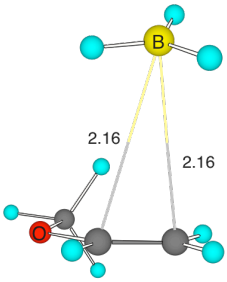
6c-6‡



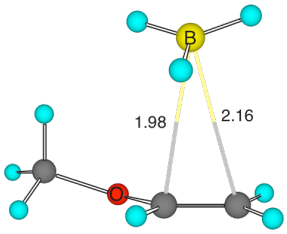
6c-7



6c-8



6c-13‡



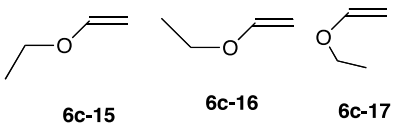
6c-14‡

Table 6.7. Enthalpies and free energies of structures located for the hydroboration of methyl vinyl ether with BH_3.

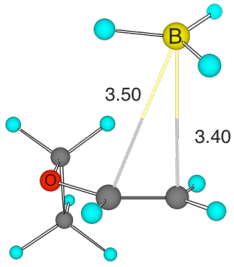
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6c-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
6c-2	$\Delta G = 1.0$ $\Delta H = 2.1$	$\Delta G = 0.8$ $\Delta H = 2.3$	$\Delta G = 0.1$ $\Delta H = 2.0$
6c-3‡	$\Delta G^{\ddagger} = 2.4$ $\Delta H^{\ddagger} = -8.8$	$\Delta G^{\ddagger} = 4.2$ $\Delta H^{\ddagger} = -8.8$	$\Delta G^{\ddagger} = 5.8$ $\Delta H^{\ddagger} = -7.2$
6c-4‡	$\Delta G^{\ddagger} = 0.6$ $\Delta H^{\ddagger} = -9.9$	$\Delta G^{\ddagger} = 1.6$ $\Delta H^{\ddagger} = -4.9$	$\Delta G^{\ddagger} = 9.6$ $\Delta H^{\ddagger} = -3.1$
6c-5‡	$\Delta G^{\ddagger} = 10.8$ $\Delta H^{\ddagger} = -0.6$	$\Delta G^{\ddagger} = 12.7$ $\Delta H^{\ddagger} = -0.37$	$\Delta G^{\ddagger} = 14.0$ $\Delta H^{\ddagger} = -1.1$
6c-6‡	$\Delta G^{\ddagger} = 6.7$ $\Delta H^{\ddagger} = -4.6$	$\Delta G^{\ddagger} = 8.4$ $\Delta H^{\ddagger} = -4.5$	$\Delta G^{\ddagger} = 9.6$ $\Delta H^{\ddagger} = -3.2$
6c-7	$\Delta G = -0.8$ $\Delta H = -10.6$	$\Delta G = 0.5$ $\Delta H = -11.9$	$\Delta G = 2.6$ $\Delta H = -9.6$
6c-8	$\Delta G = -0.5$ $\Delta H = -10.3$	$\Delta G = 0.2$ $\Delta H = -12.0$	$\Delta G = 2.2$ $\Delta H = -10.0$
6c-9	$\Delta G = -17.8$ $\Delta H = -28.6$	$\Delta G = -15.6$ $\Delta H = -30.3$	$\Delta G = -13.0$ $\Delta H = -27.5$
6c-10	$\Delta G = -15.9$ $\Delta H = -25.4$	$\Delta G = -14.8$ $\Delta H = -27.5$	$\Delta G = -13.8$ $\Delta H = -26.3$

Table 6.7 continued.

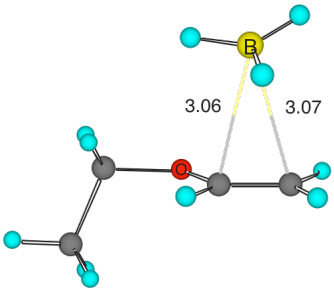
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6c-11	ΔG = - 14.6 ΔH = - 24.3	ΔG = - 13.0 ΔH = - 26.0	ΔG = - 11.7 ΔH = - 24.6
6c-12	ΔG = - 17.4 ΔH = - 26.9	ΔG = - 15.9 ΔH = - 28.9	ΔG = - 14.8 ΔH = - 27.6
6c-13‡	$\Delta G^{\ddagger}$ = 5.4 $\Delta H^{\ddagger}$ = - 2.1	$\Delta G^{\ddagger}$ = 5.7 $\Delta H^{\ddagger}$ = - 2.1	$\Delta G^{\ddagger}$ = 6.9 $\Delta H^{\ddagger}$ = - 1.3
6c-14‡	$\Delta G^{\ddagger}$ = 5.6 $\Delta H^{\ddagger}$ = - 0.4	$\Delta G^{\ddagger}$ = 5.8 $\Delta H^{\ddagger}$ = - 0.8	$\Delta G^{\ddagger}$ = 7.4 $\Delta H^{\ddagger}$ = 0



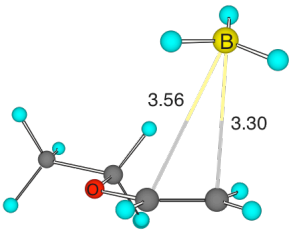
6c-15 **6c-16** **6c-17**



6c-18‡



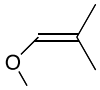
6c-19‡



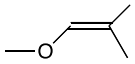
6c-20‡

Table 6.8. Enthalpies and free energies of starting material and variational transition states structures located for the hydroboration of ethyl vinyl ether with BH_3.

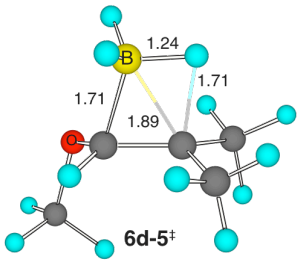
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6c-15	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
6c-16	$\Delta G = 1.2$ $\Delta H = 0.3$	$\Delta G = 3.2$ $\Delta H = 0.2$	$\Delta G = 1.6$ $\Delta H = 0.4$
6c-17	$\Delta G = 1.1$ $\Delta H = -0.4$	$\Delta G = 1.3$ $\Delta H = -0.5$	$\Delta G = 2.1$ $\Delta H = 0$
6c-18‡	$\Delta G^{\ddagger} = 6.5$ $\Delta H^{\ddagger} = -3.5$	$\Delta G^{\ddagger} = 6.9$ $\Delta H^{\ddagger} = -3.5$	$\Delta G^{\ddagger} = 8.0$ $\Delta H^{\ddagger} = -2.0$
6c-19‡	$\Delta G^{\ddagger} = 4.7$ $\Delta H^{\ddagger} = -3.7$	$\Delta G^{\ddagger} = 4.8$ $\Delta H^{\ddagger} = -4.6$	$\Delta G^{\ddagger} = 7.1$ $\Delta H^{\ddagger} = -3.0$
6c-20 ‡	$\Delta G^{\ddagger} = 4.7$ $\Delta H^{\ddagger} = -5.2$	$\Delta G^{\ddagger} = 5.0$ $\Delta H^{\ddagger} = -5.4$	$\Delta G^{\ddagger} = 5.9$ $\Delta H^{\ddagger} = -4.0$



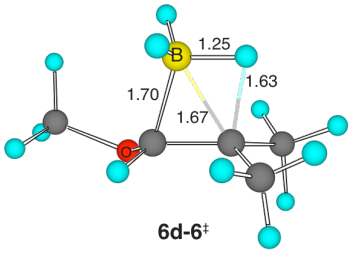
6d-1



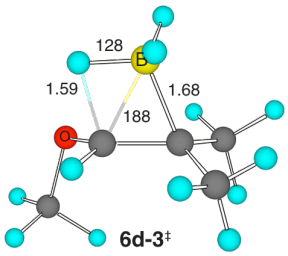
6d-2



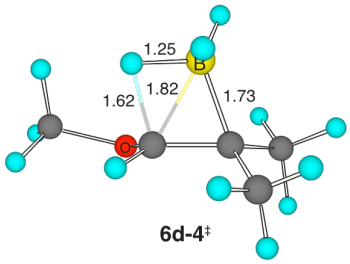
6d-5‡



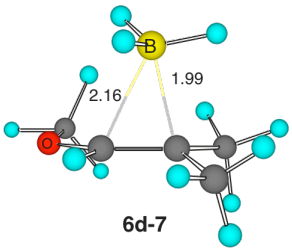
6d-6‡



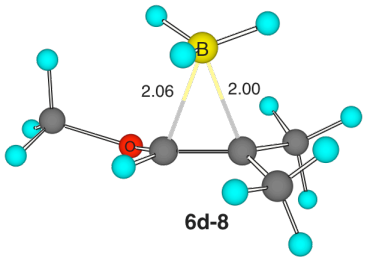
6d-3‡



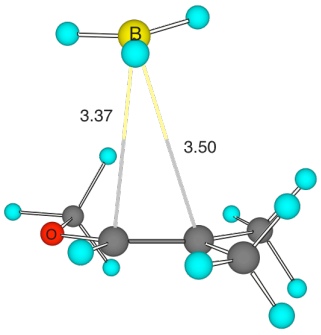
6d-4‡



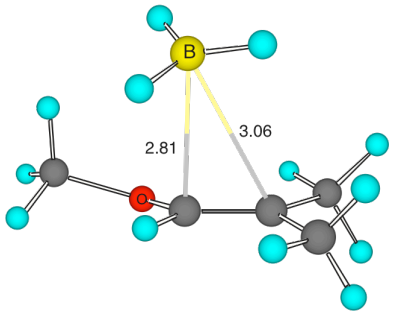
6d-7



6d-8



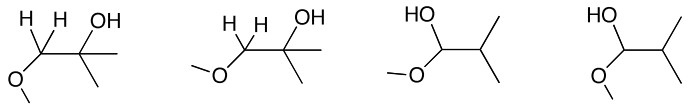
6d-14‡



6d-15‡

Table 6.9. Enthalpies and free energies of structures located for the hydroboration of isobutenyl methyl ether with BH_3.

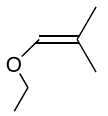
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6d-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
6d-2	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
6d-3 ‡	$\Delta G^{\ddagger} = -3.5$ $\Delta H^{\ddagger} = -14.8$	$\Delta G^{\ddagger} = 13.6$ $\Delta H^{\ddagger} = 28.4$	$\Delta G^{\ddagger} = -3.1$ $\Delta H^{\ddagger} = -16.4$
6d-4 ‡	$\Delta G^{\ddagger} = 1.1$ $\Delta H^{\ddagger} = -11.5$	$\Delta G^{\ddagger} = 22.8$ $\Delta H^{\ddagger} = 7.6$	$\Delta G^{\ddagger} = -8.7$ $\Delta H^{\ddagger} = -22.3$
6d-5 ‡	$\Delta G^{\ddagger} = 4.2$ $\Delta H^{\ddagger} = -8.3$	$\Delta G^{\ddagger} = 26.0$ $\Delta H^{\ddagger} = 11.1$	$\Delta G^{\ddagger} = -8.5$ $\Delta H^{\ddagger} = -19.1$
6d-6 ‡	$\Delta G^{\ddagger} = 1.6$ $\Delta H^{\ddagger} = -11.1$	$\Delta G^{\ddagger} = 23.5$ $\Delta H^{\ddagger} = 8.3$	$\Delta G^{\ddagger} = 11.1$ $\Delta H^{\ddagger} = -22.1$
6d-7	$\Delta G = 2.2$ $\Delta H = -9.1$	$\Delta G = 24.0$ $\Delta H = 9.0$	$\Delta G = -6.7$ $\Delta H = -20.3$
6d-8	$\Delta G = -3.5$ $\Delta H = -14.8$	$\Delta G = 17.7$ $\Delta H = 2.9$	$\Delta G = -13.3$ $\Delta H = -26.4$
6d-14‡	$\Delta G^{\ddagger} = 8.1$ $\Delta H^{\ddagger} = 1.8$	$\Delta G^{\ddagger} = 26.1$ $\Delta H^{\ddagger} = 17.7$	$\Delta G^{\ddagger} = -4.0$ $\Delta H^{\ddagger} = -12.1$
6d-15 ‡	$\Delta G^{\ddagger} = 4.3$ $\Delta H^{\ddagger} = -6.4$	$\Delta G^{\ddagger} = 22.3$ $\Delta H^{\ddagger} = 10.4$	$\Delta G^{\ddagger} = -9.5$ $\Delta H^{\ddagger} = -19.4$

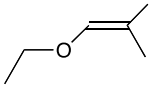


6d-10 **6d-12** **6d-11** **6d-9**

Table 6.10. Enthalpies and free energies of structures located for the products of the hydroboration of isobutenyl methyl ether with BH_3.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6d-9	ΔG = - 10.3 ΔH = - 21.7	ΔG = 11.1 ΔH = - 4.7	ΔG = - 20.5 ΔH = - 34.7
6d-10	ΔG = - 13.3 ΔH = - 25.3	ΔG = 9.7 ΔH = - 6.8	ΔG = - 21.7 ΔH = - 36.6
6d-11	ΔG = - 11.6 ΔH = - 22.5	ΔG = 9.4 ΔH = - 5.8	ΔG = - 22.2 ΔH = - 35.8
6d-12	ΔG = - 16.6 ΔH = - 29.1	ΔG = 6.2 ΔH = - 11.2	ΔG = - 24.3 ΔH = - 38.1
6d-13	ΔG = - 27.4 ΔH = - 15.4	ΔG = 6.7 ΔH = - 10.6	ΔG = - 24.0 ΔH = - 39.6


6e-1


6e-2


6e-3

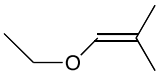
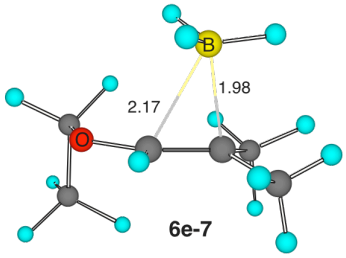
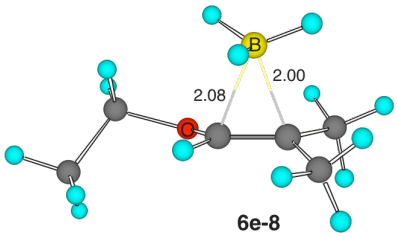

6e-4

Table 6.11. Enthalpies and free energies of structures located for the complexes and starting material of the hydroboration of isobutenyl ethyl ether with BH_3.

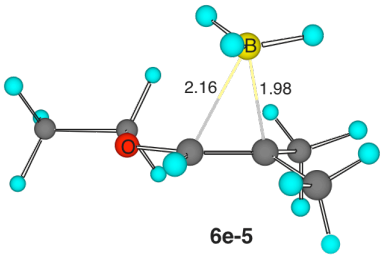
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6e-1	ΔG = 4.4 ΔH = 4.9	ΔG = 4.7 ΔH = 4.9	ΔG = 6.9 ΔH = 5.2
6e-2	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0
6e-3	ΔG = 6.7 ΔH = 6.3	ΔG = 7.5 ΔH = 6.7	ΔG = 7.8 ΔH = 7.1
6e-4	ΔG = 0.4 ΔH = 0.2	ΔG = 0.5 ΔH = 0.3	ΔG = 0.8 ΔH = 0.6
6e-5	ΔG = 2.0 ΔH = - 9.4	ΔG = 7.7 ΔH = - 6.6	ΔG = 9.5 ΔH = - 4.9
6e-6	ΔG = - 3.8 ΔH = - 15.0	ΔG = 1.2 ΔH = - 12.6	ΔG = 2.8 ΔH = - 11
6e-7	ΔG = 4.5 ΔH = - 7.0	ΔG = 10.3 ΔH = - 4.3	ΔG = 12.2 ΔH = - 2.4
6e-8	ΔG = - 2.7 ΔH = - 13.8	ΔG = 2.4 ΔH = - 11.4	ΔG = 4.0 ΔH = - 9.7



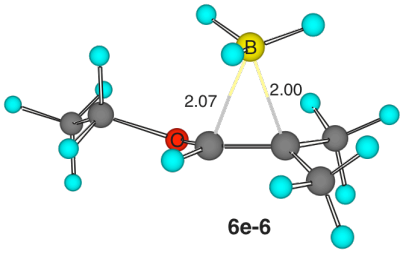
6e-7



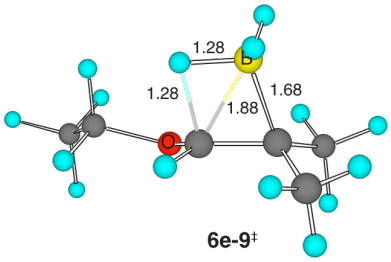
6e-8



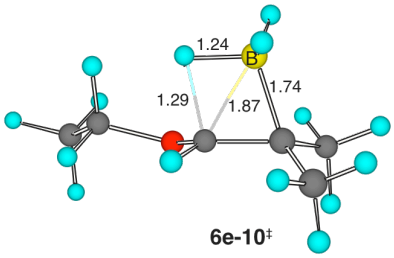
6e-5



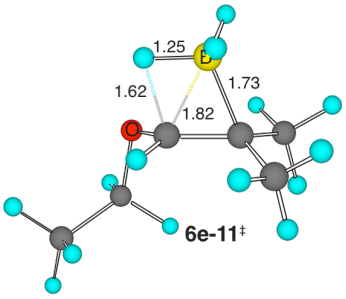
6e-6



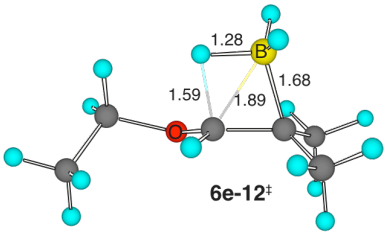
6e-9‡



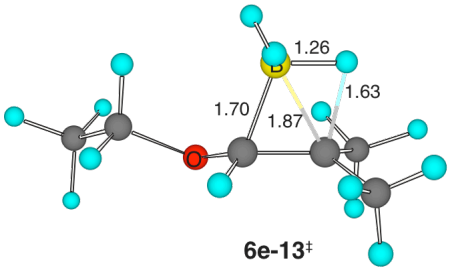
6e-10‡



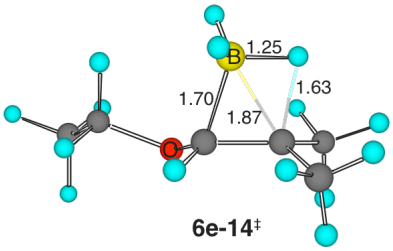
6e-11‡



6e-12‡



6e-13‡



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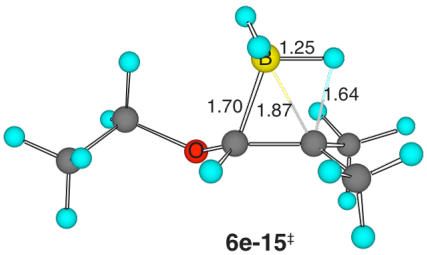

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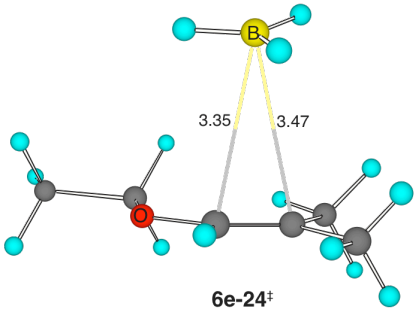

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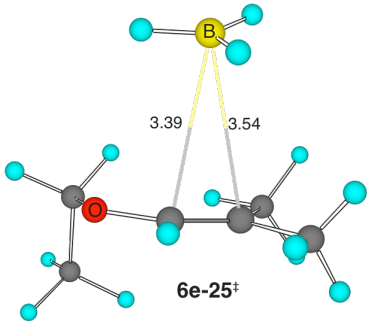

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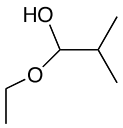
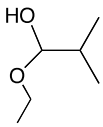


6e-19



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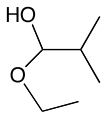

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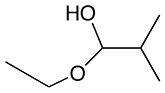

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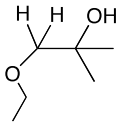

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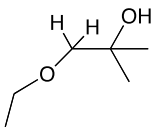

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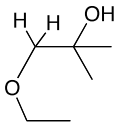

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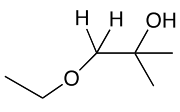


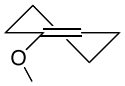
6e-21

Table 6.12. Enthalpies and free energies of structures located for the transition states of the hydroboration of isobutenyl ethyl ether with BH_3.

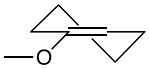
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6e-9 ‡	$\Delta G^{\ddagger}$ = 0.7 $\Delta H^{\ddagger}$ = - 11.8	$\Delta G^{\ddagger}$ = 6.3 $\Delta H^{\ddagger}$ = - 7.9	$\Delta G^{\ddagger}$ = 7.3 $\Delta H^{\ddagger}$ = - 7.0
6e-10‡	$\Delta G^{\ddagger}$ = 0.7 $\Delta H^{\ddagger}$ = - 11.8	$\Delta G^{\ddagger}$ = 6.3 $\Delta H^{\ddagger}$ = - 7.9	$\Delta G^{\ddagger}$ = 7.3 $\Delta H^{\ddagger}$ = - 7.0
6e-11‡	$\Delta G^{\ddagger}$ = 6.9 $\Delta H^{\ddagger}$ = - 5.3	$\Delta G^{\ddagger}$ = 13.3 $\Delta H^{\ddagger}$ = - 0.8	$\Delta G^{\ddagger}$ = 7.0 $\Delta H^{\ddagger}$ = - 5.3
6e-12‡	$\Delta G^{\ddagger}$ = 1.9 $\Delta H^{\ddagger}$ = - 10.5	$\Delta G^{\ddagger}$ = 7.5 $\Delta H^{\ddagger}$ = - 6.7	$\Delta G^{\ddagger}$ = 8.7 $\Delta H^{\ddagger}$ = - 5.6
6e-13‡	$\Delta G^{\ddagger}$ = 1.5 $\Delta H^{\ddagger}$ = - 11.9	$\Delta G^{\ddagger}$ = 7.3 $\Delta H^{\ddagger}$ = - 7.0	$\Delta G^{\ddagger}$ = 7.8 $\Delta H^{\ddagger}$ = - 6.5
6e-14‡	$\Delta G^{\ddagger}$ = 1.5 $\Delta H^{\ddagger}$ = - 11.1	$\Delta G^{\ddagger}$ = 7.3 $\Delta H^{\ddagger}$ = - 8.1	$\Delta G^{\ddagger}$ = 7.8 $\Delta H^{\ddagger}$ = - 6.5
6e-15 ‡	$\Delta G^{\ddagger}$ = 2.7 $\Delta H^{\ddagger}$ = - 9.9	$\Delta G^{\ddagger}$ = 8.5 $\Delta H^{\ddagger}$ = - 6.7	$\Delta G^{\ddagger}$ = 9.2 $\Delta H^{\ddagger}$ = - 5.1
6e-24‡	$\Delta G^{\ddagger}$ = 12.2 $\Delta H^{\ddagger}$ = 3.3	$\Delta G^{\ddagger}$ = 11.5 $\Delta H^{\ddagger}$ = 2.1	$\Delta G^{\ddagger}$ = 7.1 $\Delta H^{\ddagger}$ = - 3.0
6e-25 ‡	$\Delta G^{\ddagger}$ = 14.6 $\Delta H^{\ddagger}$ = 5.4	$\Delta G^{\ddagger}$ = 13.7 $\Delta H^{\ddagger}$ = 4.3	$\Delta G^{\ddagger}$ = 5.9 $\Delta H^{\ddagger}$ = - 4.0

Table 6.13. Enthalpies and free energies of structures located for the products of the hydroboration of isobutenyl ethyl ether with BH_3.

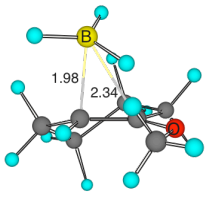
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6e-16	ΔG = - 11.7 ΔH = - 22.6	ΔG = - 6.8 ΔH = - 21.2	ΔG = - 5.7 ΔH = - 20.1
6e-17	ΔG = - 10.3 ΔH = - 21.1	ΔG = - 5.2 ΔH = - 19.6	ΔG = - 4.0 ΔH = - 18.4
6e-18	ΔG = - 11.7 ΔH = - 22.6	ΔG = - 6.8 ΔH = - 21.2	ΔG = - 5.7 ΔH = - 20.1
6e-19	ΔG = - 5.7 ΔH = - 20.1	ΔG = - 6.8 ΔH = - 21.2	ΔG = - 11.7 ΔH = - 22.6
6e-20	ΔG = - 13.5 ΔH = - 25.7	ΔG = - 6.6 ΔH = - 22.4	ΔG = 5.9 ΔH = - 4.0
6e-21	ΔG = - 12.4 ΔH = - 23.4	ΔG = - 6.6 ΔH = - 21.3	ΔG = - 5.5 ΔH = - 20.2
6e-22	ΔG = - 13.5 ΔH = - 25.7	ΔG = - 6.6 ΔH = - 22.4	ΔG = - 7.9 ΔH = - 22.5
6e-23	ΔG = 13.9 ΔH = - 24.9	ΔG = - 8.0 ΔH = - 22.7	ΔG = - 7.0 ΔH = - 21.8



6f-1



6f-2



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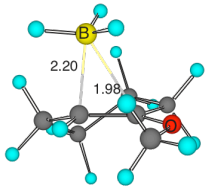

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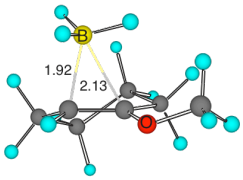

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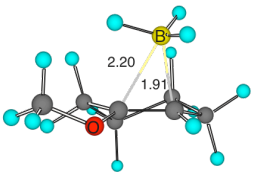
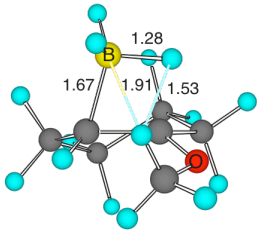
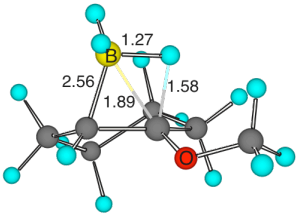


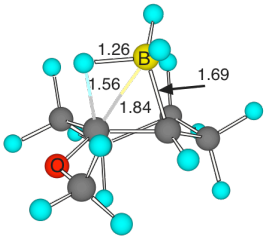
6f-6



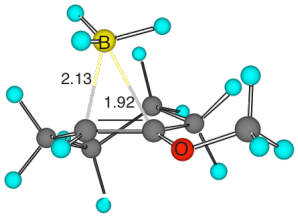
6f-7‡



6f-9‡



6f-8‡



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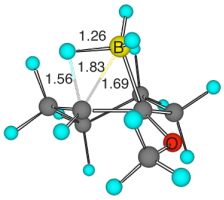

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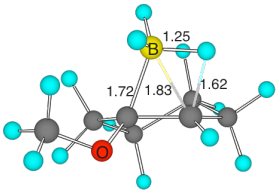

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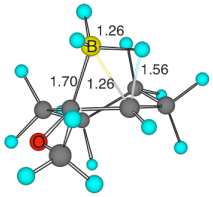

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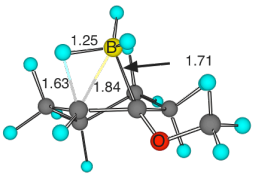


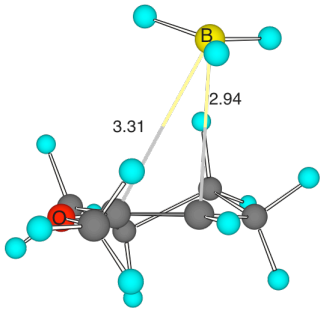
6f-13‡

Table 6.14. Enthalpies and free energies of structures located for the products of the hydroboration of methoxycyclohexene with BH_3.

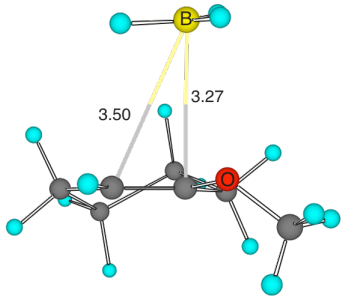
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6f-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
6f-2	$\Delta G = 3.7$ $\Delta H = 4.4$	$\Delta G = 3.5$ $\Delta H = 4.4$	$\Delta G = 3.6$ $\Delta H = 4.4$
6f-3	$\Delta G = -2.1$ $\Delta H = -12.7$	$\Delta G = 2.5$ $\Delta H = -10.8$	$\Delta G = 4.0$ $\Delta H = -9.2$
6f-4	$\Delta G = -2.1$ $\Delta H = -12.7$	$\Delta G = 2.5$ $\Delta H = -10.8$	$\Delta G = 4.0$ $\Delta H = -9.2$
6f-5	$\Delta G = 0.2$ $\Delta H = -10.2$	$\Delta G = 4.8$ $\Delta H = -8.2$	$\Delta G = 6.4$ $\Delta H = -6.5$
6f-6	$\Delta G = 0.3$ $\Delta H = -10.1$	$\Delta G = 4.4$ $\Delta H = -8.5$	$\Delta G = 6.1$ $\Delta H = -6.8$
6f-7 ‡	$\Delta G^{\ddagger} = 4.0$ $\Delta H^{\ddagger} = -7.6$	$\Delta G^{\ddagger} = 9.9$ $\Delta H^{\ddagger} = -3.1$	$\Delta G^{\ddagger} = 10.7$ $\Delta H^{\ddagger} = -2.8$
6f-8 ‡	$\Delta G^{\ddagger} = 11.5$ $\Delta H^{\ddagger} = -0.3$	$\Delta G^{\ddagger} = 17.3$ $\Delta H^{\ddagger} = 3.7$	$\Delta G^{\ddagger} = 17.8$ $\Delta H^{\ddagger} = 4.3$
6f-9 ‡	$\Delta G^{\ddagger} = 3.0$ $\Delta H^{\ddagger} = -8.8$	$\Delta G^{\ddagger} = 8.7$ $\Delta H^{\ddagger} = -4.8$	$\Delta G^{\ddagger} = 9.6$ $\Delta H^{\ddagger} = -3.8$
6f-10	$\Delta G = 0.2$ $\Delta H = -10.2$	$\Delta G = 8.6$ $\Delta H = -4.7$	$\Delta G = 9.4$ $\Delta H = -3.8$

Table 6.14 continued.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6f-11‡	$\Delta G^{\ddagger} = 11.5$ $\Delta H^{\ddagger} = -0.3$	$\Delta G^{\ddagger} = 17.3$ $\Delta H^{\ddagger} = 3.7$	$\Delta G^{\ddagger} = 17.8$ $\Delta H^{\ddagger} = 4.3$
6f-12‡	$\Delta G^{\ddagger} = 12.3$ $\Delta H^{\ddagger} = 0.4$	$\Delta G^{\ddagger} = 17.8$ $\Delta H^{\ddagger} = 4.3$	$\Delta G^{\ddagger} = 18.4$ $\Delta H^{\ddagger} = 4.9$
6f-13‡	$\Delta G^{\ddagger} = 8.2$ $\Delta H^{\ddagger} = -3.7$	$\Delta G^{\ddagger} = 13.7$ $\Delta H^{\ddagger} = 0.1$	$\Delta G^{\ddagger} = 14.3$ $\Delta H^{\ddagger} = 0.8$
6f-14‡	$\Delta G^{\ddagger} = 8.8$ $\Delta H^{\ddagger} = -3.0$	$\Delta G^{\ddagger} = 14.2$ $\Delta H^{\ddagger} = 0.8$	$\Delta G^{\ddagger} = 14.9$ $\Delta H^{\ddagger} = 1.5$



6f-29‡



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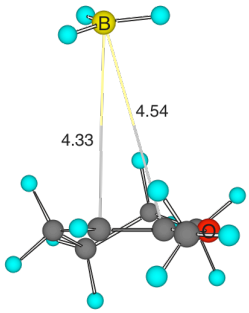
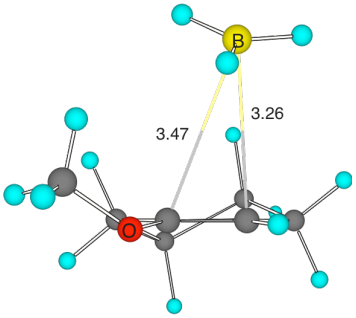


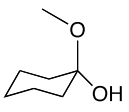
6f-27‡



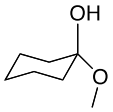
6f-30‡

Table 6.15. Enthalpies and free energies of structures located for the entropic association barriers in the hydroboration of methyl vinyl ether with BH_3.

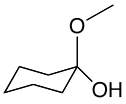
Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6f-27 ‡	$\Delta G^{\ddagger}$ = 5.0 $\Delta H^{\ddagger}$ = - 1.4	$\Delta G^{\ddagger}$ = 6.0 $\Delta H^{\ddagger}$ = - 0.6	$\Delta G^{\ddagger}$ = 5.9 $\Delta H^{\ddagger}$ = - 0.3
6f-28 ‡	$\Delta G^{\ddagger}$ = 7.8 $\Delta H^{\ddagger}$ = 0.3	$\Delta G^{\ddagger}$ = 9.8 $\Delta H^{\ddagger}$ = 1.7	$\Delta G^{\ddagger}$ = 5.9 $\Delta H^{\ddagger}$ = - 0.3
6f-29 ‡	$\Delta G^{\ddagger}$ = 7.8 $\Delta H^{\ddagger}$ = 0.2	$\Delta G^{\ddagger}$ = 34.7 $\Delta H^{\ddagger}$ = - 4.6	$\Delta G^{\ddagger}$ = 27.0 $\Delta H^{\ddagger}$ = 15.8
6f-30 ‡	$\Delta G^{\ddagger}$ = 7.8 $\Delta H^{\ddagger}$ = 0.2	$\Delta G^{\ddagger}$ = 9.3 $\Delta H^{\ddagger}$ = 0.9	$\Delta G^{\ddagger}$ = 10.7 $\Delta H^{\ddagger}$ = 2.0



6f-15



6f-16



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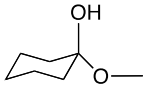

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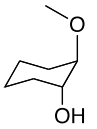

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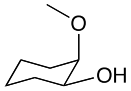
6f-20



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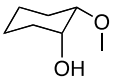

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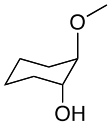

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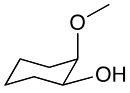

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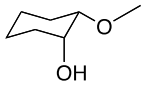
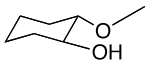


6f-24



6f-26

Table 6.16. Enthalpies and free energies of structures located for the products from the hydroboration of methoxycyclohexene with BH_3.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6f-15	ΔG = - 10.9 ΔH = - 21.8	ΔG = - 5.1 ΔH = - 19.5	ΔG = - 3.8 ΔH = - 18.0
6f-16	ΔG = - 9.4 ΔH = - 20.3	ΔG = - 3.8 ΔH = - 18.0	ΔG = - 2.8 ΔH = - 17.0
6f-17	ΔG = - 10.9 ΔH = - 21.8	ΔG = - 5.1 ΔH = - 19.5	ΔG = - 3.9 ΔH = - 18.0
6f-18	ΔG = - 9.4 ΔH = - 20.3	ΔG = - 3.8 ΔH = - 18.0	ΔG = - 2.8 ΔH = - 17.0
6f-19	ΔG = - 14.1 ΔH = - 24.8	ΔG = - 8.6 ΔH = - 22.5	ΔG = - 7.7 ΔH = - 21.5
6f-20	ΔG = - 14.0 ΔH = - 25.2	ΔG = - 8.6 ΔH = - 23.3	ΔG = - 7.6 ΔH = - 22.2
6f-21	ΔG = - 10.8 ΔH = - 22.8	ΔG = - 4.6 ΔH = - 20.8	ΔG = - 2.7 ΔH = - 18.8
6f-22	ΔG = - 13.0 ΔH = - 23.5	ΔG = - 7.8 ΔH = - 21.4	ΔG = - 6.8 ΔH = - 20.3
6f-23	ΔG = - 13.8 ΔH = - 24.4	ΔG = - 8.5 ΔH = - 22.3	ΔG = - 7.6 ΔH = - 21.3

Table 6.16 continued.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6f-24	ΔG = - 14.6 ΔH = - 24.5	ΔG = - 9.9 ΔH = - 23.4	ΔG = - 8.6 ΔH = - 22.3
6f-25	ΔG = - 16.2 ΔH = - 27.9	ΔG = - 30.6 ΔH = - 42.5	ΔG = 11.0 ΔH = - 5.8
6f-26	ΔG = - 13.3 ΔH = - 23.5	ΔG = - 8.0 ΔH = - 21.4	ΔG = - 7.1 ΔH = - 20.5

For all systems, matching to previous cases, because the consideration of whether transition state theory is making accurate predictions often hinges on relatively small energy differences, second-order perturbative anharmonic contributions to the vibrational energies and entropy were calculated[85] for each transition state, complex and starting material, structure and applied as corrections for enthalpies and free energy. The resulting energetics for this system after these corrections are summarized in Tables **6.17** to **6.21**.

Table 6.17. Enthalpies and free energies of structures located for the hydroboration of methyl vinyl ether with BH_3 after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6c-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
6c-2	$\Delta G = 0.1$ $\Delta H = 2.1$	$\Delta G = 0.7$ $\Delta H = 2.3$	$\Delta G = 0.0$ $\Delta H = 2.0$
6c-3‡	$\Delta G^{\ddagger} = 2.1$ $\Delta H^{\ddagger} = -8.8$	$\Delta G^{\ddagger} = 3.9$ $\Delta H^{\ddagger} = -8.8$	$\Delta G^{\ddagger} = 5.5$ $\Delta H^{\ddagger} = -7.2$
6c-4‡	$\Delta G^{\ddagger} = 0.0$ $\Delta H^{\ddagger} = -9.9$	$\Delta G^{\ddagger} = 1.0$ $\Delta H^{\ddagger} = -4.9$	$\Delta G^{\ddagger} = 9.0$ $\Delta H^{\ddagger} = -3.1$
6c-5‡	$\Delta G^{\ddagger} = 10.2$ $\Delta H^{\ddagger} = -0.5$	$\Delta G^{\ddagger} = 12.1$ $\Delta H^{\ddagger} = -0.37$	$\Delta G^{\ddagger} = 13.4$ $\Delta H^{\ddagger} = -1.1$
6c-6‡	$\Delta G^{\ddagger} = 6.3$ $\Delta H^{\ddagger} = -4.6$	$\Delta G^{\ddagger} = 7.8$ $\Delta H^{\ddagger} = -4.5$	$\Delta G^{\ddagger} = 9.2$ $\Delta H^{\ddagger} = -3.2$
6c-7	$\Delta G = -1.4$ $\Delta H = -10.6$	$\Delta G = 0.1$ $\Delta H = -11.9$	$\Delta G = 2.0$ $\Delta H = -9.6$
6c-8	$\Delta G = -1.2$ $\Delta H = -10.3$	$\Delta G = 0.5$ $\Delta H = -12.0$	$\Delta G = 1.5$ $\Delta H = -10.0$

Table 6.18. Enthalpies and free energies of starting material and complex structures located for the hydroboration of isobutenyl methyl ether with BH_3 after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6d-1	ΔG = -0.1 ΔH =0.8	ΔG = - 0.1 ΔH =0.8	ΔG = - 0.1 ΔH = 0.8
6d-2	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0
6d-3 ‡	$\Delta G^{\ddagger}$ = - 4.4 $\Delta H^{\ddagger}$ = - 15.5	$\Delta G^{\ddagger}$ = 12.7 $\Delta H^{\ddagger}$ = 27.6	$\Delta G^{\ddagger}$ = - 4.0 $\Delta H^{\ddagger}$ = - 17.1
6d-4 ‡	$\Delta G^{\ddagger}$ = 0.6 $\Delta H^{\ddagger}$ = - 11.7	$\Delta G^{\ddagger}$ = 22.4 $\Delta H^{\ddagger}$ = 7.4	$\Delta G^{\ddagger}$ = - 9.2 $\Delta H^{\ddagger}$ = - 22.5
6d-5 ‡	$\Delta G^{\ddagger}$ = 4.2 $\Delta H^{\ddagger}$ = - 8.3	$\Delta G^{\ddagger}$ = 26.0 $\Delta H^{\ddagger}$ = 11.1	$\Delta G^{\ddagger}$ = - 8.5 $\Delta H^{\ddagger}$ = - 19.1
6d-6 ‡	$\Delta G^{\ddagger}$ = 1.4 $\Delta H^{\ddagger}$ = - 11.8	$\Delta G^{\ddagger}$ = 23.3 $\Delta H^{\ddagger}$ = 7.6	$\Delta G^{\ddagger}$ = 11.0 $\Delta H^{\ddagger}$ = - 22.8
6d-7	ΔG = 1.5 ΔH = - 10.0	ΔG = 23.3 ΔH = 8.1	ΔG = - 7.4 ΔH = - 21.2
6d-8	ΔG = - 5.2 ΔH = - 14.6	ΔG = 19.4 ΔH = 2.7	ΔG = - 15.0 ΔH = - 26.2

Table 6.19. Enthalpies and free energies of starting material and complex structures located for the hydroboration of isobutenyl ethyl ether with BH_3 after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6e-1	ΔG = 5.7 ΔH = 6	ΔG = 6.0 ΔH = 6	ΔG = 8.2 ΔH = 6.3
6e-2	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0	ΔG = 0 ΔH = 0
6e-3	ΔG = 7.4 ΔH = 7.4	ΔG = 8.2 ΔH = 7.8	ΔG =8.5 ΔH =8.24
6e-4	ΔG = 0.4 ΔH = 1.0	ΔG = 1.1 ΔH = 0.7	ΔG = 1.4 ΔH = 1
6e-5	ΔG = 1.1 ΔH = - 9.7	ΔG = 6.8 ΔH = - 6.7	ΔG = 8.6 ΔH = - 5.2
6e-6	ΔG = - 4.5 ΔH = - 15.6	ΔG = 0.5 ΔH = - 13.2	ΔG = 2.1 ΔH = - 11.6
6e-7	ΔG = 3.9 ΔH = - 7.4	ΔG = 9.7 ΔH = - 4.7	ΔG = 11.6 ΔH = - 2.8
6e-8	ΔG = - 3.0 ΔH = - 13.1	ΔG = 2.1 ΔH = - 10.7	ΔG = 3.7 ΔH = - 9

Table 6.20. Enthalpies and free energies of transition state structures located for the hydroboration of isobutenyl ethyl ether with BH_3 after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6e-9 ‡	$\Delta G^{\ddagger}$ = 1.1 $\Delta H^{\ddagger}$ = - 11.4	$\Delta G^{\ddagger}$ = 6.7 $\Delta H^{\ddagger}$ = - 7.5	$\Delta G^{\ddagger}$ = 7.7 $\Delta H^{\ddagger}$ = - 7.4
6e-10‡	$\Delta G^{\ddagger}$ = 1.1 $\Delta H^{\ddagger}$ = - 11.4	$\Delta G^{\ddagger}$ = 6.7 $\Delta H^{\ddagger}$ = - 7.5	$\Delta G^{\ddagger}$ = 7.3 $\Delta H^{\ddagger}$ = - 7.3
6e-11‡	$\Delta G^{\ddagger}$ = 7.4 $\Delta H^{\ddagger}$ = - 5.6	$\Delta G^{\ddagger}$ = 13.9 $\Delta H^{\ddagger}$ = - 0.4	$\Delta G^{\ddagger}$ = 7.6 $\Delta H^{\ddagger}$ = - 1.2
6e-12‡	$\Delta G^{\ddagger}$ = 1.7 $\Delta H^{\ddagger}$ = - 10.9	$\Delta G^{\ddagger}$ = 7.3 $\Delta H^{\ddagger}$ = - 7.1	$\Delta G^{\ddagger}$ = 8.5 $\Delta H^{\ddagger}$ = - 6.0
6e-13‡	$\Delta G^{\ddagger}$ = 1.5 $\Delta H^{\ddagger}$ = - 11.7	$\Delta G^{\ddagger}$ = 7.4 $\Delta H^{\ddagger}$ = - 6.8	$\Delta G^{\ddagger}$ = 7.9 $\Delta H^{\ddagger}$ = - 6.3
6e-14‡	$\Delta G^{\ddagger}$ = 1.8 $\Delta H^{\ddagger}$ = - 10.9	$\Delta G^{\ddagger}$ = 7.4 $\Delta H^{\ddagger}$ = - 7.9	$\Delta G^{\ddagger}$ = 7.9 $\Delta H^{\ddagger}$ = - 6.3
6e-15‡	$\Delta G^{\ddagger}$ = 2.8 $\Delta H^{\ddagger}$ = - 9.9	$\Delta G^{\ddagger}$ = 86 $\Delta H^{\ddagger}$ = - 6.7	$\Delta G^{\ddagger}$ = 9.3 $\Delta H^{\ddagger}$ = - 5.1

Table 6.21. Enthalpies and free energies of structures located for the hydroboration of methoxycyclohexene with BH_3 after anharmonic corrections.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6f-1	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$	$\Delta G = 0$ $\Delta H = 0$
6f-2	$\Delta G = 3.8$ $\Delta H = 3.1$	$\Delta G = 3.6$ $\Delta H = 3.1$	$\Delta G = 3.7$ $\Delta H = 3.1$
6f-3	$\Delta G = -3.0$ $\Delta H = -12.8$	$\Delta G = 1.6$ $\Delta H = -10.7$	$\Delta G = 3.1$ $\Delta H = -9.3$
6f-4	$\Delta G = -3.1$ $\Delta H = -12.7$	$\Delta G = 1.5$ $\Delta H = -10.8$	$\Delta G = 3.0$ $\Delta H = -9.2$
6f-5	$\Delta G = -0.7$ $\Delta H = -10.3$	$\Delta G = 3.9$ $\Delta H = -8.3$	$\Delta G = 5.5$ $\Delta H = -6.6$
6f-6	$\Delta G = -1.4$ $\Delta H = -10.2$	$\Delta G = 2.7$ $\Delta H = -8.6$	$\Delta G = 4.4$ $\Delta H = -6.7$
6f-7 ‡	$\Delta G^{\ddagger} = 3.7$ $\Delta H^{\ddagger} = -7.6$	$\Delta G^{\ddagger} = 9.6$ $\Delta H^{\ddagger} = -3.1$	$\Delta G^{\ddagger} = 10.4$ $\Delta H^{\ddagger} = -2.8$
6f-8 ‡	$\Delta G^{\ddagger} = 10.7$ $\Delta H^{\ddagger} = -0.4$	$\Delta G^{\ddagger} = 16.5$ $\Delta H^{\ddagger} = 3.8$	$\Delta G^{\ddagger} = 17$ $\Delta H^{\ddagger} = 4.4$
6f-9 ‡	$\Delta G^{\ddagger} = 3.3$ $\Delta H^{\ddagger} = -8.8$	$\Delta G^{\ddagger} = 9.0$ $\Delta H^{\ddagger} = -4.8$	$\Delta G^{\ddagger} = 9.9$ $\Delta H^{\ddagger} = -3.8$

Table 6.21 continued.

Structure	g3b3	B3LYP/6-31G*	B3LYP/6-31+G**
6f-11‡	$\Delta G^{\ddagger}$ = 10.7 $\Delta H^{\ddagger}$ = - 0.4	$\Delta G^{\ddagger}$ = 16.5 $\Delta H^{\ddagger}$ = 3.6	$\Delta G^{\ddagger}$ = 17.0 $\Delta H^{\ddagger}$ = 4.2
6f-12‡	$\Delta G^{\ddagger}$ = 12.3 $\Delta H^{\ddagger}$ = 0.3	$\Delta G^{\ddagger}$ = 17.8 $\Delta H^{\ddagger}$ = 4.2	$\Delta G^{\ddagger}$ = 18.4 $\Delta H^{\ddagger}$ = 4.8
6f-13‡	$\Delta G^{\ddagger}$ = 8.0 $\Delta H^{\ddagger}$ = - 3.8	$\Delta G^{\ddagger}$ = 13.5 $\Delta H^{\ddagger}$ = 0.0	$\Delta G^{\ddagger}$ = 14.1 $\Delta H^{\ddagger}$ = 0.1
6f-14‡	$\Delta G^{\ddagger}$ = 8.3 $\Delta H^{\ddagger}$ = - 3.1	$\Delta G^{\ddagger}$ = 13.7 $\Delta H^{\ddagger}$ = 0.7	$\Delta G^{\ddagger}$ = 14.4 $\Delta H^{\ddagger}$ = 1.4

We calculated the transition structures leading to the regioisomeric products of the reaction of methyl vinyl ether/ BH_3 in order to determine if the theoretical path compares to other systems where dynamic effects explain the selectivity. The G3B3 $\Delta\Delta G^{\ddagger}$ between **6c-4**‡ and **6c-6**‡ is 6.3 kcal/mol after corrections. The calculated free energy association barriers, variational transition structures located **6c-13**‡-**6c-14**‡, were 5.4-5.6 kcal/mol. This is 0.9 kcal/mol lower in free energy than Markovnikov transition structure **6c-5**‡. Under these circumstances, only considering the energetics of the system, we can predict that is a case of dynamics and transition state theory being in accidental agreement. We suggest dynamics due to the similarities of the energetics to the hydroboration of 2-methyl-2-butene with BH_3 system discussed in Chapter IV.

Consideration of the reaction energetics insinuates the capability of dynamic effect to predict the product ratio. The formation of **6c-8** from BH_3 / methyl vinyl ether is enthalpically barrierless and downhill by 8.2 kcal/mol as shown in Figure **6.3**. Considerable excess energy is thus available from the formation of **6c-8**, and the barriers for formation of product **6c-10** and **6c-12** from **6c-8** is quite small. Transition state **6c-4**‡ is only 1.4 kcal/mol above π-complex **6c-8** in free energy and 0.3 kcal/mol above π-complex **6c-8** in enthalpy. Under these circumstances, we considered that trajectories may pass to product 6c-**10** and **6c-12** faster than thermal equilibration with solvent.

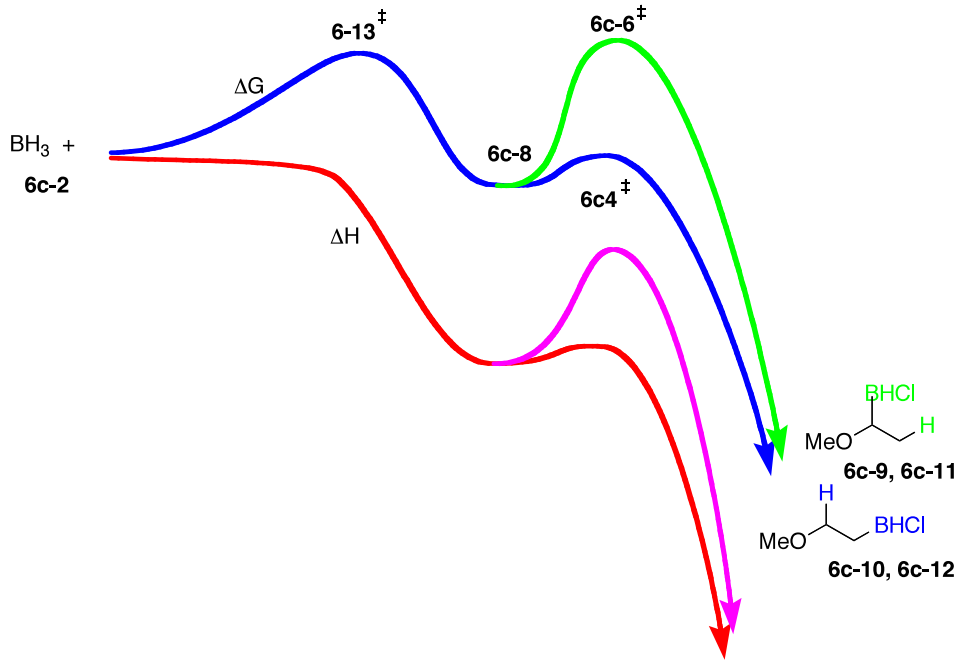


Figure 6.3. Free energy and enthalpy reaction coordinate diagram for the hydroboration of methyl vinyl ether with BH_3, representing the lowest energy conformation for each point.

The hydroboration of isobutenyl ethyl ether with BH_3 in THF afforded 100% of the anti-Markovnikov product experimentally. We calculated the transition structures leading to the regioisomeric products for the hydroboration of isobutenyl ethyl ether and isobutenyl methyl ether with BH_3 in order to compare if the predicted $\Delta\Delta G^{\ddagger}$ corresponds to the experimental results. The G3B3 $\Delta\Delta G^{\ddagger}$ between **6d-4**‡ and **6d-6**‡, the lowest conformation transition states leading to the two regioisomeric product for the hydroboration of isobutenyl methyl ether is ~0.8 kcal/mol after corrections. The free energy association barriers, variational transition structures **6d-14**‡-**6d-15**‡, were 8.1-4.3 kcal/mol. This is 2.9 kcal/mol higher in free energy than transition structure **6d-6**‡, which leads to a product where the boron attaches to the least substituted carbon, the carbon alpha to the oxygen (**6d-11**).

The G3B3 $\Delta\Delta G^{\ddagger}$ between **6e-9**‡ and **6e-13**‡, the lowest conformation transition states leading to the two regioisomeric products for the hydroboration of isobutenyl ethyl ether is ~0.4 kcal/mol after corrections. However, when we allowed for the contribution of all the conformations to the ratio, according to the free energy the experimental ratio predicted was 73:27. A 73% for the transition states leading to products **4e-20, 4e-21 4e-22** and **4e-23** (**6e-9**‡-**6e-12**‡, leads to product where the boron attaches to the more substituted carbon, the carbon beta to the oxygen) and a 27 % for the transition states leading to products**, 4e-17 4e-18** and **4e-19** (**6e-13**‡-**6e-15**‡, leads to product where the boron attaches to the least substituted carbon, the carbon alpha to the oxygen). We should mention that a transition state leading to **4e-16** corresponding to a conformation from starting material **6e-3** was not located. However we predict that the energy should

be very high as was the case for the similar conformation for opposite transition state **6e-11**‡, due to the difficulties finding it.

Taking into account each of these conformations for both cases, isobutenyl methyl ether and isobutenyl ethyl ether, in the predicted $\Delta\Delta G^{‡}$ for the transition states leading to the regioisomeric products, suggests the inability of transition state theory to account for the product ratio. To find an explanation for the product ratio it was necessary to pay close attention to the reaction energetics. Figure **6.4** shows the enthalpic and free-energy profile for the hydroboration of isobutenyl ethyl ether with BH_3.

As previously found with propene, there is no enthalpic barrier for formation of the olefin – BH_3 π-complexes **6d-7** and **6e-6** from separate isobutenyl methyl ether or isobutenyl ethyl ether and BH_3 molecules. This is downhill by ~15 kcal/mol for the case of isobutenyl ethyl ether and 4 kcal/mol for isobutenyl methyl ether/ BH_3. The free energy association barriers, variational transition structures **6e-24**‡ and **6d-15**‡, were 9.7 and 4.3 kcal/mol. Under these circumstances, considering only the energetics of the system, we can predict that this is a case of dynamics.

Consideration of the reaction energetics insinuates the capability of dynamic effect to predict the product ratio. The formation of **6d-7** from BH_3 / isobutenyl methyl ether is enthalpically barrierless and downhill by 4 kcal/mol and the formation of **6e-6** from BH_3 / isobutenyl ethyl ether is enthalpically barrierless and downhill by 15 kcal/mol. Significant excess energy is thus available from the formation of **6d-7** or **6e-6** in each case, and the barriers for formation of products from **6d-7** or **6e-6** are quite small. Transition state **6d-4**‡ is only 0.8 kcal/mol above π-complex **6d-7** in free energy and 1.7

kcal/mol above π-complex **6d-7** in enthalpy. Transition states **6e-9**‡ and **6e-10**‡ are about 5 kcal/mol above π-complex **6e-6** in free energy and 4.2 kcal/mol above π-complex **6e-6** in enthalpy. Under these circumstances, we considered that trajectories may pass to product faster than thermal equilibration with solvent.

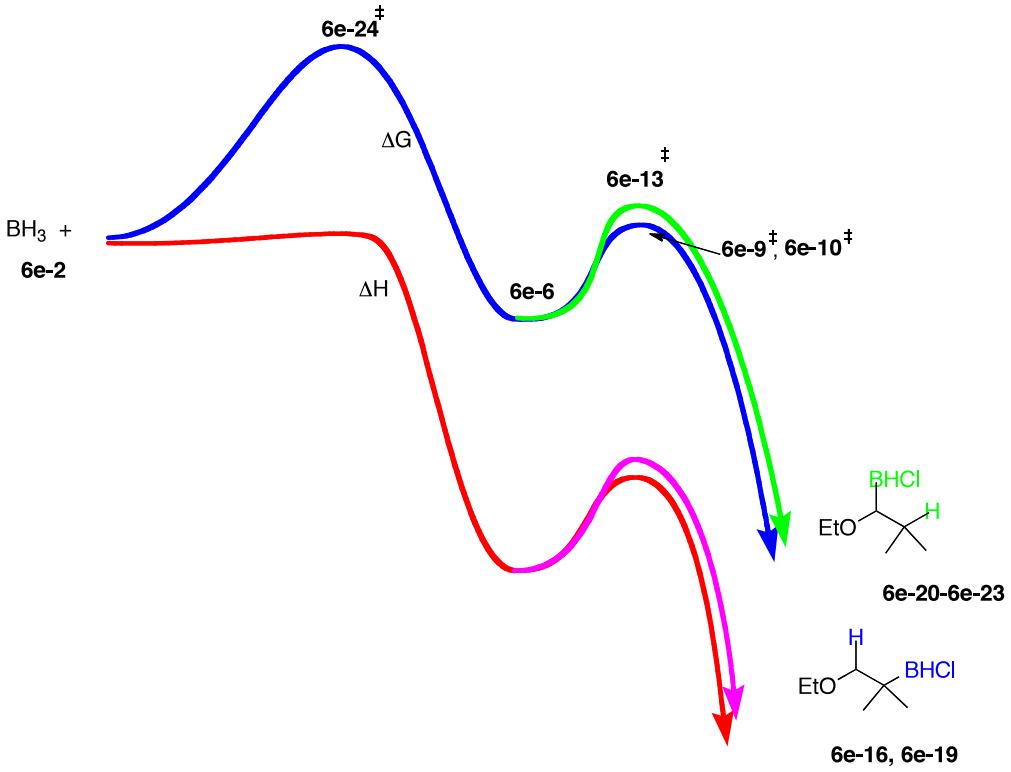


Figure 6.4. Free energy and enthalpy reaction coordinate diagram for the hydroboration of isobutenyl ethyl ether with BH_3, representing the lowest energy conformation for each point.

As well as isobutenyl ethyl ether, the hydroboration of methoxycyclohexene with BH_3 in THF afforded 100% of the anti-Markovnikov product experimentally.[24] We calculated the transition structures leading to the regioisomeric products in order to

compare if the predicted $\Delta\Delta G^{\ddagger}$ corresponds to the experimental results. The G3B3 $\Delta\Delta G^{\ddagger}$ between **6f-9**‡ and **6f-13**‡ is ~4.7 kcal/mol after corrections. This translates to a predicted selectivity of 100% for the anti-Markovnikov form considering all possible conformation and facial attacks. The free energy association barriers, variational transition structures **6f-27**‡-**6f-30**‡, were 5.0-7.8 kcal/mol. This is 2.0 kcal/mol lower than Markovnikov transition structure **6f-13**‡, showing similar results to 2-methyl-2-butene. On the other hand, the formation of π-complex **6f-3**, the lowest in energy is downhill by ~11.4 kcal/mol from **6f-27**‡, the lowest energy variational transition state (Figure **6.5**). Looking at the regioselectivity, a dynamic control process still has to cross-differing heights of barriers in order to get to a completive form of product. Under those circumstances it is easy to envision an accidental agreement of transition state theory with experiment.

Summarizing the findings from the theoretical paths calculated for representative cases for the hydroboration of chloro and ethoxy functional derivative alkenes, we found an entropic association barrier for the formation of the π-complex in all cases. It was determined for the allylchloride and ethoxy functional alkenes cases that the formation of such π-complex is enthalpically barrierless. Dynamics cases were established, when the enthalpic association barrier found was the rate-limiting step and the barrier for the formation of products from π-complex were small. For chlorocyclohexene, the results were inconclusive. Whereas for the hydroboration of methoxycyclohexene and vinyl methyl ether with BH_3, similar to the case of 2-methyl-2-butene, we suggested an accidental agreement of transition state theory with experiment.

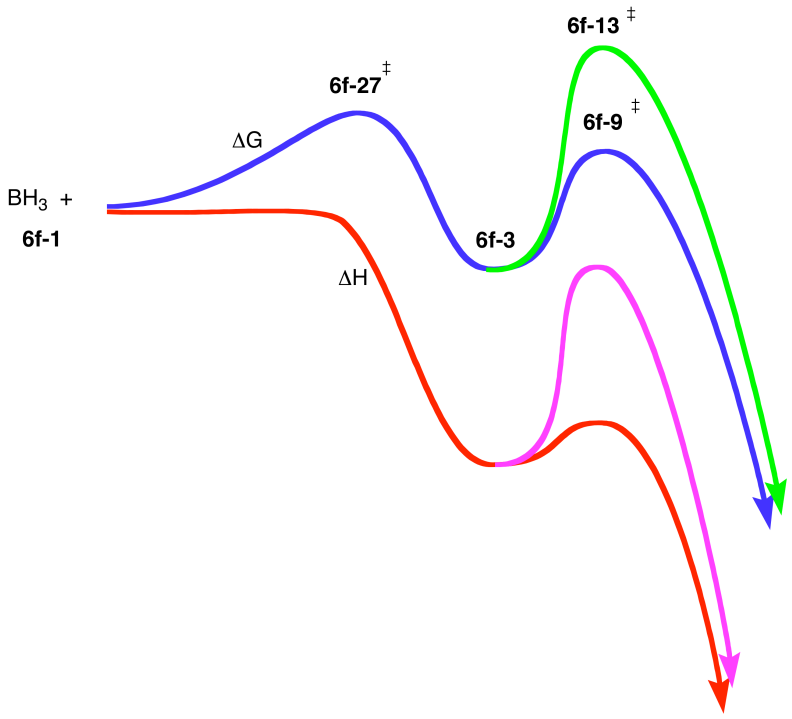


Figure 6.5. Free energy and enthalpy reaction coordinate diagram for the hydroboration of methoxycyclohexene with BH_3, representing the lowest energy conformation for each point.

CHAPTER VII

EXPERIMENTAL AND CALCULATIONAL PROCEDURES

General Calculational Procedures

Calculations employed either Gaussian03,[104] ACESII,[105] or Gaussian09.[106] Default procedures in Gaussian03 and Gaussian09 were employed unless otherwise noted. When ACESII was used, the options were set to mimic the default values in Gaussian03 and checks were performed to ensure comparable results from the two programs. Full structures and energetics are provided in a section below.

The program suite PROGDYN used for dynamics is listed at the end of the appendix as a series of component programs as either Unix shell scripts or awk programs. Gaussian03 was used to calculate the forces at each point in trajectories.[104]

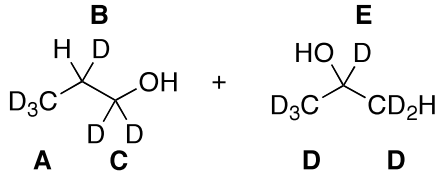
Some minor variations in the subprogram *proganal* of PROGDYN were used to accomplish the "equilibrated" trajectories. For the trajectories equilibrated 500 fs before releasing the fixed B-C distance, *proganal* was reprogrammed to make a change in progdyn.conf automatically after 500 fs eliminating the fixed distance. For the trajectories involving 500 – 8500 fs equilibrations, *proganal* was reprogrammed to save starting conditions at 500 fs intervals. Series of these starting conditions were used to initiate new trajectories with no fixed distances.

Experimental Procedures for 'Dynamics and the Failure of Transition State Theory in the Hydroboration of Terminal Alkenes with BH_3'

General. Oven-dried or flame-dried glassware was cooled under a stream of nitrogen prior to use, and standard syringe-and-septa techniques were employed in all cases. ^2H NMR chemical shifts were assigned relative to the natural abundance deuterium in THF at δ 3.727 or water at δ 4.4.

Hydroboration of Propene-d_6 (100 equiv BH_3; 21 °C). To 270 mL (270 mmol) of 1 M borane in THF at 21 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d6 (at -48 °C) by cannula. After stirring 6 h at 21 °C, the mixture was cooled to 0 °C and 85 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 45-min period. The resulting mixture was allowed to warm to room temperature and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at d 3.92, 3.48, 1.52, 1.14, 0.89 were assigned to positions E, C, B, D, and A in the 1,1,2,3,3,3-hexadeutero-1-propanol and 1,1,1,2,3,3-hexadeutero-2-propanol products as shown below. Integrations of 373.5, 154.4, 267.6, 67.2, and 21.7 were observed for peaks A, B, C, D, and E, respectively.

Scheme 7.1



Independent Hydroboration of Propene-d_6 (100 equiv BH_3; 21 °C). To 270 mL (270 mmol) of 1 M borane in THF at 21 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 6 h at 21 °C, the mixture was cooled to 0 °C and 85 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 45-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at δ 3.92, 3.48, 1.52, 1.14, 0.89 were assigned to positions E, C, B, D, and A in the 1,1,2,3,3,3-hexadeutero-1-propanol and 1,1,1,2,3,3-hexadeutero-2-propanol products as shown below. Integrations of 98.91, 18.40, 37.41, 70.31, and 4.67 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene-d_6 (100 equiv BH_3; 70 °C). To 270 mL (270 mmol) of 1 M borane in THF at 70 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 2 h at 70 °C, the mixture was cooled to 0 °C and 85 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 45-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at δ 3.92, 3.48, 1.52, 1.14, 0.89 were assigned to positions E, C, B, D, and A in the 1,1,2,3,3,3-hexadeutero-1-propanol and 1,1,1,2,3,3-hexadeutero-2-propanol products as shown below. Integrations of 569.5, 197.8, 364.3, 118.1, and 24.0 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene-d_6 (100 equiv BH_3; 45 °C). To 270 mL (270 mmol) of 1 M borane in THF at 45 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 2 h at 45 °C, the mixture was cooled to 0 °C and 85 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 45-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). The ^{2}H NMR peaks at δ 3.92, 3.48, 1.52, 1.14, 0.89 were assigned to positions E, C, B, D, and A in the 1,1,2,3,3,3-hexadeutero-1-propanol and 1,1,1,2,3,3-hexadeutero-2-propanol products as shown below. Integrations of 580.4, 198.8, 389.8, 113.1, and 26.1 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene-d_6 (0.3 equiv BH_3; 21 °C). To 0.9 mL (0.9 mmol) of 1 M borane in THF at 21 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 6 h at 21 °C, the mixture was cooled to 0 °C and 1 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 15-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by ^{2}H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 1000, 69.7, 309.4, 650.4, and 12.7 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene-d_6 (44 equiv BH_3; 21 °C). To 118.9 mL (118.9 mmol) of 1 M borane in THF at 21 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 6 h at 21 °C, the mixture

was cooled to 0 °C and 69.2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 1000, 334.6, 668.3, 134.2, and 28.6 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene-d_6 (37 equiv BH_3; 70 °C). To 100 mL (100 mmol) of 1 M borane in THF at 70 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 2 h at 70 °C, the mixture was cooled to 21 °C stirred for 1.5 h, then the reaction mixture was cooled to 0 °C and 32 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 20-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). Integrations of 1000, 345.5, 657.7, 156.5, and 32.6 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene-d_6 (37 equiv BH_3; 48 °C). To 100 mL (100 mmol) of 1 M borane in THF at 48 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 0.5 h at 48 °C, the mixture was cooled to 21 °C stirred for 2 h, then the reaction mixture was cooled to 0 °C and 31 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 20-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by

^{2}H NMR. Integrations of 950.024, 139.904, 307.1, 589.051, and 24.858, were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene-d_6 (37 equiv BH_3; -6 °C). To 100 mL (100 mmol) of 1 M borane in THF at -6 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 162 h at -6 °C, a 20 mL aliquot of the mixture was added dropwise by syringe over a 20-min period to another round bottom flask containing 14 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 at 0 °C. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). Integrations of 1000, 345.5, 657.7, 156.5 and 32.6 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene-d_6 with BH_3•SMe_2 in 1,2-dichlorobenzene. To a mixture of 14.8 mL (156.05 mmol) of borane dimethyl sulfide complex and 141 mL of 1,2 dichlorobenzene at 21 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 12 h at 21 °C, the mixture was cooled to 0 °C and 49 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. The final two layers were analyzed directly by ^{2}H NMR in two different ways each. A 1-mL aliquot of the resulting aqueous solution was then analyzed directly by ^{2}H NMR (400 MHz, 10 μL pyridine-d_6). Integrations of 983.8, 327.8, 647.5, 157.5, 31.4 and 2000 were observed for peaks A, B, C, D, E, and

pyridine respectively. A second 1-mL aliquot of the aqueous solution was also analyzed directly by ^{2}H NMR (400 MHz, 10 μL Methanol-d_4). Integrations of 617.7, 203.1, 428.0, 92.6, 17.5, and 3000 were observed for peaks A, B, C, D, E, and methanol-CH_3 respectively. A 1-mL aliquot of the organic layer was also analyzed directly by ^{2}H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 239.3, 81.1, 157.2, 27.8, 4.8, and 100 were observed for peaks A, B, C, D, E, and $CDCl_3$ respectively. A second 1-mL aliquot of the same organic solution was also analyzed directly by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). Integrations of 122.2, 41.2, 80.5, 12.7, 1.9, and 100 were observed for peaks A, B, C, D, E, and $CDCl_3$ respectively

Hydroboration of Propene-d_6 with BH_3•SMe_2 in diglyme. To a mixture of 11.27 mL (118.8 mmol) of borane dimethyl sulfide complex and 118.9 mL of diethylene glycol dimethyl ether at 21 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 12 h at 21 °C, the mixture was cooled to 0 °C and 60 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting aqueous solution was then analyzed directly by ^{2}H NMR (400 MHz, 10 μL pyridine-d_6) at 75 °C. Integrations of 1000, 351.4, 619.5, 108.7, and 14.7 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of Propene- d_6 with BH_3•SMe_2 Neat. To 11.27 mL (118.8 mmol) of borane dimethyl sulfide complex at 21 °C was added 0.25 mL (130 mg, 2.7

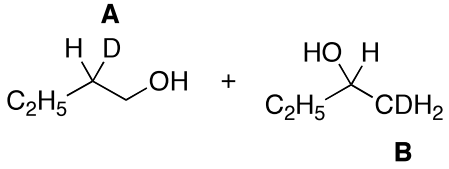
mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 8 h at 21 °C, the mixture was cooled to 0 °C and 50 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting aqueous solution was then analyzed directly by ^{2}H NMR (400 MHz, 10 μL pyridine-d_6). Integrations of 784.69, 263.9, 522.4, 84.5, and 14.9 were observed for peaks A, B, C, D, and E, respectively.

Repeated Hydroboration of Propene-d_6 with BH_3•SMe_2 Neat. To 11.27 mL (118.8 mmol) of borane dimethyl sulfide complex at 21 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 8 h at 21 °C, the mixture was cooled to 0 °C and 60 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. A 1-mL aliquot of the resulting aqueous solution was then analyzed directly by ^{2}H NMR (400 MHz, 10 μL pyridine-d_6). Integrations of 1000, 335.9, 666.0, 103.5, and 16.2 were observed for peaks A, B, C, D, and E, respectively.

Hydroboration of 1-butene (3 equiv of BD_3). To 1 mL (1 mmol) of 1 M borane-d_3 in THF complex solution at 21 °C was added 31 μL (19 mg, 0.33 mmol) of condensed 1-butene (at -6.3 °C) by cannula. After stirring 4 h at 21 °C, the mixture was cooled to 0 °C and 0.5 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 5-min period. The reaction mixture was allowed to warm to 21 °C and was stirred overnight. To the resulting solution, 1.2 mL of $CHCl_3$ and

1.2 mL of water were added. The organic layer was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). The ^{2}H NMR peaks at δ 1.63 and 1.27 were assigned to positions A and B in the 2-deutero-1-butanol and 1-deutero-2-butanol products as shown below. Integrations of 3705.5 and 196.6 were observed for peaks A and B respectively. The hydroboration of 1-butene at 21 °C with 3 equiv of BD_3•THF affords 5.0:95.0 ratio of primary to secondary alcohols after oxidation.

Scheme 7.2



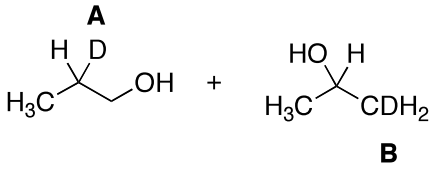
Hydroboration of 1-butene (0.3 equiv of BD_3). To 1 mL (1 mmol) of 1 M borane-d_3 in THF complex solution at 21 °C was added 0.28 mL (167 mg, 3 mmol) of condensed 1-butene (at -6.3 °C) by cannula. After stirring 6 h at 21 °C, the mixture was cooled to 0 °C and 0.5 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 5-min period. The reaction mixture was allowed to warm to 21 °C and was stirred overnight. To the resulting solution, 1.2 mL of $CHCl_3$ and 1.2 mL of water were added. The organic layer was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). Integrations of 5334.8 and 218.6 were observed for peaks A and B respectively. The hydroboration of 1-butene at 21 °C with 0.3 equiv of BD_3•THF affords 3.9:96.1 ratio of primary to secondary alcohols after oxidation.

Independent Hydroboration of 1-butene (3 equiv of BD_3). To 2 mL (2 mmol) of 1 M borane-d_3 in THF complex solution at 21 °C was added 62 μL (37 mg, 0.66 mmol) of condensed 1-butene (at -6.3 °C) by cannula. After stirring for 12 h at 21 °C, the mixture was cooled to 0 °C and 0.6 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 5-min period. The reaction mixture was allowed to warm to 21 °C and was stirred overnight. To the resulting solution, 1.2 mL of $CHCl_3$ and 1.2 mL of water were added. The organic layer was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). Integrations of 760 and 45 were observed for peaks A and B respectively. The hydroboration of 1-butene at 21 °C with 3 equiv of BD_3•THF affords 5.6:94.4 ratio of primary to secondary alcohols after oxidation.

Hydroboration of Propene (Organic layer in $CHCl_3$ analysis). To 1 mL (1 mmol) of 1 M borane-d_3 in THF at 21 °C was added 26 μL (24 mg, 0.57 mmol) of condensed propene (at -48 °C) by cannula. After stirring 6 h at 21 °C, the mixture was cooled to 0 °C and 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. To the resulting solution 2 mL of $CHCl_3$ and 5 mL of water were added, the organic layer was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at δ 1.66 and 1.29 were assigned to positions A and B in the 2-deutero-1-propanol and 1-deutero-2-propanol products as shown below. Integrations of 1188.5 and 44.9 were observed for peaks A and B respectively. The organic layer in $CDCl_3$ from the

hydroboration of propene at 21 °C with 1.8 equiv of BD_3•THF affords 3.6:96.4 ratio of primary to secondary alcohols after oxidation.

Scheme 7.3



Independent Hydroboration of Propene (Direct analysis). To 1 mL (1 mmol) of 1 M borane-d_3 in THF at 21 °C was added 26 μL (24 mg, 0.57 mmol) of condensed propene (at -48 °C) by cannula. After stirring 6 h at 21 °C, the mixture was cooled to 0 °C and 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. The resulting solution was then analyzed directly by ^{2}H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 2303.6 and 86.0 were observed for peaks A and B respectively. The direct analysis of the hydroboration of propene at 21 °C with 1.8 equiv of BD_3•THF affords 3.6:96.4 ratio of primary to secondary alcohols after oxidation.

Hydroboration of Propene (Organic layer in EtOAc analysis). To 1 mL (1 mmol) of 1 M borane-d_3 in THF at 21 °C was added 26 μL (24 mg, 0.57 mmol) of condensed propene (at -48 °C) by cannula. After stirring 6 h at 21 °C, the mixture was cooled to 0 °C and 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min

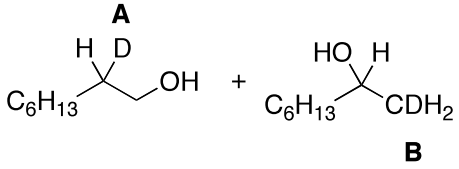
period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. To the resulting solution 2 mL of EtOAc were added, the organic layer was then analyzed directly by ^{2}H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 968.3 and 55.2 were observed for peaks A and B respectively. The organic layer in ethyl acetate from the hydroboration of propene at 21 °C with 1.8 equiv of BD_3•THF affords 5.4:94.6 ratio of primary to secondary alcohols after oxidation.

Hydroboration of Propene (6.7 equiv of BD_3). To 1 mL (1 mmol) of 1 M borane-d_3 in THF at 21 °C was added 12 μL (6.2 mg, 0.15 mmol) of condensed propene (at -48 °C) by cannula. After stirring for 12 h at 21 °C, the mixture was cooled to 0 °C and 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. To the resulting solution, 1.2 mL of $CHCl_3$ were added. The organic layer was then analyzed directly by ^{2}H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 869.6 and 107.9 were observed for peaks A and B respectively. The hydroboration of propene at 21 °C with 6.7 equiv of BD_3•THF affords 11.0:89.0 ratio of primary to secondary alcohols after oxidation.

Hydroboration of Octene (3 equiv of BD_3). To 1 mL (1 mmol) of 1 M borane-d_3 in THF at 21 °C was added 47 mL (34 mg, 0.3 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.5 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution, 1.2 mL of $CHCl_3$ and 1.2 mL of water were

added. The organic layer was then analyzed by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). The ^{2}H NMR peaks at d 1.54 and 1.16 were assigned to positions A and B in the 2-deutero-1-octanol and 1-deutero-2-octanol products as shown below. Integrations of 3665.4 and 157.0 were observed for peaks A and B respectively. The hydroboration of octene at 21 °C with 3 equiv of BD_3•THF affords 4.1:95.9 ratio of primary to secondary alcohols after oxidation.

Scheme 7.4



Independent Hydroboration of Octene (3 equiv of BD_3). To 0.9 mL (0.9 mmol) of 1 M borane-d_3 in THF at 21 °C was added 47 μL (34 mg, 0.3 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution, 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. The resulting light yellow oil was dissolved in 1.2 mL of $CHCl_3$ and analyzed by ^{2}H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 1530 and 106.8 were observed for peaks A and B respectively. The hydroboration of octene at 21 °C with 3 equiv of BD_3•THF affords 6.5:93.4 ratio of primary to secondary alcohols after oxidation.

Hydroboration of Octene (15 equiv of BD_3). To 1 mL (1 mmol) of 1 M borane-d_3 in THF at 21 °C was added 10.4 μL (7.5 mg, 0.07 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution, 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. The resulting light yellow oil was dissolved in 1.2 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 315 and 20.1 were observed for peaks A and B respectively.

Independent Hydroboration of Octene (15 equiv of BD_3). To 1 mL (1 mmol) of 1 M borane-d_3 in THF at 21 °C was added 10.4 μL (7.5 mg, 0.07 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution, 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. The resulting light yellow oil (9.6 mg) was dissolved in 1.2 mL of $CHCl_3$ and analyzed by (400 MHz, 10 μL $CDCl_3$). Integrations of 561.5 and 20.2 were observed for peaks A and B respectively.

Hydroboration of Octene (3 equiv of BD_3). To 0.9 mL (0.9 mmol) of 1 M borane-d_3 in THF at 21 °C was added 47 μL (34 mg, 0.3 mmol) of octene by syringe. After stirring for 12 h at 21°C, 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a

5-min period. The resulting mixture was stirred overnight. To the reaction solution, 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. From resulting light yellow oil 17 mg were dissolved in 1.2 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 390.0 and 27.0 were observed for peaks A and B respectively. The hydroboration of octene at 21 °C with 3 equiv of BD_3•THF affords 6.5:93.5 ratio of primary to secondary alcohols after oxidation.

Independent Hydroboration of Octene (3 equiv of BD_3). To 1 mL (1 mmol) of 1 M borane-d_3 in THF at 21 °C was added 52 μL (37 mg, 0.3 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.3 mL of a of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution, 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. From resulting light yellow oil 32.2 mg were dissolved in 2 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 1440 and 91.5 were observed for peaks A and B respectively. The hydroboration of octene at 21 °C with 3 equiv of BD_3•THF affords 6.0:94.0 ratio of primary to secondary alcohols after oxidation.

Hydroboration of Octene (15 equiv of BD_3). To 4 mL (4 mmol) of 1 M borane-d_3 in THF at 21 °C was added 42 μL (30 mg, 0.27 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 1.2 mL of a of 3 M NaOH in water was added dropwise over a 20-min period and 1.2 mL of 30% H_2O_2 in water was then added dropwise over a

10-min period. The resulting mixture was stirred overnight. To the reaction solution, 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. From resulting light yellow oil 22.9 mg were dissolved in 2 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 1320.1 and 123.9 were observed for peaks A and B respectively.

Hydroboration of Octene (55 equiv of BH_3; -6 °C). To 100 mL (100 mmol) of 1 M borane in THF at 21 °C was added 286 μL (204 mg, 1.8 mmol) of octene *via* syringe. After stirring 14 h at 21 °C, 25 mL of a of 3 M NaOH in water was added dropwise over a 40-min period at 21 °C and 25 mL of 30% H_2O_2 in water was then added dropwise over a 30-min period. The resulting mixture was stirred 12 h at 21 °C. To the reaction solution, 30 mL of ether and 30 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. The resulting light yellow oil was analyzed by GC. The ratio in area % were 12.38 to 87.62 for 2-octanol to 1-octanol respectively.

Hydroboration of Octene (55 equiv of BH_3; -6 °C). To 100 mL (100 mmol) of 1 M borane in THF at -6 °C was added 286 μL (204 mg, 1.8 mmol) of octene *via* syringe. After stirring for 120 h in the freezer at -6 °C, 25 mL of a of 3 M NaOH in water was added dropwise over a 40-min period at -6 °C and 25 mL of 30% H_2O_2 in water was then added dropwise over a 30-min period. The resulting mixture was stirred 12 h at 21 °C. To the reaction solution, 30 mL of ether and 30 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. The resulting

light yellow oil was analyzed by GC. The ratio in area % were 11.95 to 88.05 for 2-octanol to 1-octanol respectively.

Independent Hydroboration of Octene (55 equiv of BH_3; -6 °C). To 100 mL (100 mmol) of 1 M borane in THF at -6 °C was added 286 μL (204 mg, 1.8 mmol) of octene *via* syringe. After stirring 1 week in freezer at -6 °C, 25 mL of a of 3 M NaOH in water was added dropwise over a 40-min period at -6 °C and 25 mL of 30% H_2O_2 in water was then added dropwise over a 30-min period. The resulting mixture was stirred 12 h at 21 °C. To the reaction solution, 30 mL of ether and 30 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. The resulting light yellow oil was analyzed by GC. The ratio in area % were 12.16 to 87.86 for 2-octanol to 1-octanol respectively.

Stock Solution of 9:1 H:D Borane. A stock solution of 1 M borane in THF containing a mixture of hydrogen and deuterium was prepared by mixing 9 mL of 1 M BH_3 in THF with 1 mL of 1 M BD_3 in THF. The stock solution of borane prepared from mixtures of BH_3 and BD_3 was allowed to equilibrate at 21 °C for 48 h.

To allow for the departure of this solution from a precisely 9:1 ratio of H:D, the same stock solution was used to prepare isotopic the "standard" (where no isotopic fractionation had occurred) and the "sample" (prepared under conditions in which isotopic fractionation occurs).

Isotopic "Standard" in the Hydroboration of Octene with 9:1 H:D Borane. To 4.5 mL (4.5 mmol) of the stock solution of 9:1 H:D borane at 21 °C was added 2.1 mL (1.5 g, 13.5 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 1.5 mL of a

solution of 3 M NaOH in water was added dropwise over a 20-min period and 1.5 mL of 30% H_2O_2 in water was then added dropwise over a 10-min period. The resulting mixture was stirred overnight. To the reaction solution 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. From resulting light yellow oil 50.6 mg were dissolved in 1.2 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 175.2, 12.0 and 1000 were observed for peaks A, B and $CDCl_3$ respectively.

Hydroboration of Octene with 9:1 H:D Borane. To 4.5 mL (4.5 mmol) of the stock solution of 9:1 H:D borane at 21 °C was added 235 μL (168 mg, 1.5 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 1.5 mL of a solution of 3 M NaOH in water was added dropwise over a 20-min period and 1.5 mL of 30% H_2O_2 in water was then added dropwise over a 10-min period. The resulting mixture was stirred overnight. To the reaction solution 5 mL of $CHCl_3$ and 5 mL of water were added, the organic layer was then dried over sodium sulfate and concentrated. The resulting light yellow oil (50.4 mg) were dissolved in 1.2 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 161.1, 10.7 and 1000 were observed for peaks A, B and $CDCl_3$ respectively.

Independent Stock Solution of 9:1 H:D Borane. A stock solution of 1 M borane in THF containing a mixture of hydrogen and deuterium was prepared by mixing 9 mL of 1 M BH_3 in THF with 1 mL of 1 M BD_3 in THF. The stock solution of borane prepared from mixtures of BH_3 and BD_3 was allowed to equilibrate at 22 °C for 24 h.

To allow for the departure of this solution from a precisely 9:1 ratio of H:D, the same stock solution was used to prepare the isotopic "standard" (where no isotopic fractionation had occurred) and the "sample" (prepared under conditions in which isotopic fractionation occurs).

Hydroboration of Octene with 9:1 H:D Borane. To 4 mL (4 mmol) of the resulting stock solution of 9:1 H:D borane at 21 °C was added 1.9 mL (1.3 g, 12 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 1.2 mL of a solution of 3 M NaOH in water was added dropwise over a 20-min period and 1.2 mL of 30% H_2O_2 in water was then added dropwise over a 10-min period. The resulting mixture was stirred overnight. To the reaction solution 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. From resulting light yellow oil 50.6 mg were dissolved in 1.2 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 180.9, 11.8 and 1000 were observed for peaks A, B and $CDCl_3$ respectively.

Isotopic "Standard" in the Hydroboration of Octene with 9:1 H:D Borane. To 4.5 mL (4.5 mmol) of the resulting stock solution of 1:1 H:D borane at 21 °C was added 235 μL (168 mg, 1.5 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 1.5 mL of a solution of 3 M NaOH in water was added dropwise over a 20-min period and 1.5 mL of 30% H_2O_2 in water was then added dropwise over a 10-min period. The resulting mixture was stirred overnight. To the reaction solution 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. The resulting light yellow oil (50.5 mg) were dissolved in 1.2 mL of

$CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 149.7, 11.7 and 1000 were observed for peaks A, B and $CHCl_3$ respectively.

Stock Solution of 1:1 H:D Borane. A stock solution of 1 M borane in THF containing an approximately equal mixture of hydrogen and deuterium was prepared by mixing 1 mL of 1 M BH_3 in THF with 1 mL of 1 M BD_3 in THF. The stock solution of borane prepared from mixtures of BH_3 and BD_3 was allowed to equilibrate at 22 °C for 24 h.

To allow for the departure of this solution from a precisely 1:1 ratio of H:D, the same stock solution was used to prepare the isotopic "standard" (where no isotopic fractionation had occurred) and the "sample" (prepared under conditions in which isotopic fractionation occurs).

Isotopic "Standard" in the Hydroboration of Octene with 1:1 H:D Borane. To 1 mL (1 mmol) of the resulting stock solution of 1:1 H:D borane at 21 °C was added 469 μL (335 mg, 3 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.3 mL of a solution of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2 in water was then added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. From resulting light yellow oil 22.3 mg were dissolved in 1.2 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 122.8, 15.4 and 1000 were observed for peaks A, B and $CHCl_3$ respectively.

"Sample" in the Hydroboration of Octene with 1:1 H:D Borane. To 1 mL (1 mmol) of the resulting stock solution of 1:1 H:D borane at 21 °C was added 52 μL (37 mg, 0.33 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.3 mL of a solution of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2in water was then added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. From resulting light yellow oil 43.2 mg were dissolved in 1.2 mL of $CHCl_3$ and analyzed by ^{2}H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 213.5, 16.2 and 1000 were observed for peaks A, B and $CHCl_3$ respectively.

Independent Stock Solution of 1:1 H:D Borane. A stock solution of 1 M borane in THF containing an approximately equal mixture of hydrogen and deuterium was prepared by mixing 2 mL of 1 M BH_3 in THF with 2 mL of 1 M BD_3 in THF. The stock solution of borane prepared from mixtures of BH_3 and BD_3 was allowed to equilibrate at 22 °C for 12 h.

Isotopic "Standard" in the Hydroboration of Octene with 1:1 H:D Borane. To 2 mL (2 mmol) of the resulting stock solution of 1:1 H:D borane at 21 °C was added 939 μL (672 mg, 6 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.6 mL of a solution of 3 M NaOH in water was added dropwise over a 15-min period and 0.6 mL of 30% H_2O_2in water was then added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and

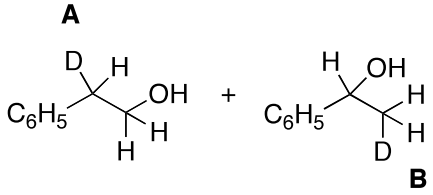
concentrated. From resulting light yellow oil 64.8 mg were dissolved in 1.5 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 398.4, 83.6 and 1000 were observed for peaks A, B and $CHCl_3$ respectively.

"Sample" in the Hydroboration of Octene with 1:1 H:D Borane. To 2 mL (2 mmol) of the resulting stock solution of 1:1 H:D borane at 21 °C was added 104 μL (74 mg, 0.67 mmol) of octene by syringe. After stirring for 12 h at 21 °C, 0.3 mL of a solution of 3 M NaOH in water was added dropwise over a 10-min period and 0.3 mL of 30% H_2O_2in water was then added dropwise over a 5-min period. The resulting mixture was stirred overnight. To the reaction solution 5 mL of $CHCl_3$ and 5 mL of water were added. The organic layer was then dried over sodium sulfate and concentrated. From resulting light yellow oil 64.5 mg were dissolved in 1.5 mL of $CHCl_3$ and analyzed by ^2H NMR (400 MHz, 10 μL $CDCl_3$). Integrations of 701.1, 30.9 and 1000 were observed for peaks A, B and $CHCl_3$ respectively.

Experimental Procedures for 'Isotope Effects, Dynamics, and the Nature of the Selectivity in the Hydroboration of Styrene'

General. Oven-dried or flame-dried glassware was cooled under a stream of nitrogen prior to use, and standard syringe-and-septa techniques were employed in all cases. ^2H NMR chemical shifts were assigned relative to the known chemical shift of the larger peak, **B** in $CDCl_3$ for ^1H NMR (400 MHz) at δ 1.53.

Scheme 7.5



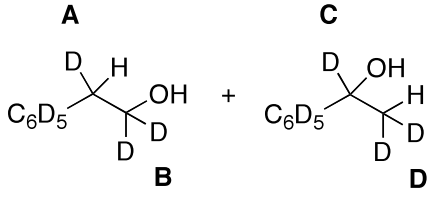
Hydroboration of Styrene (44 equiv of BD_3; 22 °C). To 10 mL (10 mmol) of 1 M borane-d_3 in THF at 22 °C was added 26 μL (23.6 mg, 0.23 mmol) of styrene by syringe. After stirring 4 h at 22 °C, the mixture was cooled to 0 °C and 3 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 5-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 3 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 4 mL of ether, then the excess solvent was removed by rotavap. The resulting solution (~1 mL) was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). The ^{2}H NMR peaks at δ 2.94, 1.53 were assigned to positions A, and B in the 2-pheny-2,-deutero-ethanol and 1-pheny-2-deutero-ethanol products as shown above. Integrations of 1000 and 240.9 were observed for peaks A and B, respectively.

Hydroboration of Styrene (0.3 equiv of BD_3; 22 °C). To 3 mL (3 mmol) of 1 M borane-d_3 in THF at 22 °C was added 1.03 mL (937 mg, 9 mmol) of styrene by syringe. After stirring 4 h at 22 °C, the mixture was cooled to 0 °C and 1.8 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 20-min period. The resulting mixture was allowed to warm to 22 °C and was stirred

overnight. To the mixture, 3 mL of ether were added and after 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was removed by rotavap. The resulting solution (~1 mL) was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at d 2.94, 1.53 were assigned to positions A, and B in the 2-pheny-2,-deutero-ethanol and 1-pheny-2-deutero-ethanol products as shown above. Integrations of 279.2 and 54.0 were observed for peaks A and B, respectively.

For all Styrene-d_8 hydroborations the ^2H NMR chemical shifts were assigned relative to the known chemical shift of the larger peak, **B** in $CDCl_3$ for ^1H NMR (400 MHz) at δ 3.83.

Scheme 7.6



Hydroboration of Styrene-d_8 (100 equiv of BH_3; 22 °C). To 10 mL (10 mmol) of 1 M borane in THF at 22 °C was added 11.6 μL (11.2 mg, 0.1 mmol) of styrene-d_8 by syringe. After stirring 4 h at 22 °C, the mixture was cooled to 0 °C and 6 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was

stirred overnight. To the mixture, 6 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 4 mL of ether, then the excess solvent was removed by rotavap. The resulting solution (~1 mL) was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at δ 4.93, 3.83, 2.94, 1.53 were assigned to positions C, B, A, and D in the 2-pentadeuterophenyl-1,1,2,-trideutero-ethanol and 1-pentadeuteropheny-l-1,2,2-trideutero-ethanol products as shown above. Integrations of 143.2, 1000, 484.0, and 287.5 were observed for peaks C, B, A, and D, respectively.

Hydroboration of Styrene-d_8 (44 equiv of BH_3; 22 °C). To 100 mL (100 mmol) of 1 M borane in THF at 22 °C was added 26.0 μL (25.5 mg, 2.3 mmol) of styrene-d_8 by syringe. After stirring 4 h at 22 °C, the mixture was cooled to 0 °C and 6 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 6 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 4 mL of ether, then the excess solvent was removed by rotavap. The resulting solution (~1 mL) was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at δ 4.93, 3.83, 2.94, 1.53 were assigned to positions C, B, A, and D in the 2-pentadeuterophenyl-1,1,2,-trideutero-ethanol and 1-pentadeuteropheny-l-1,2,2-trideutero-ethanol products as shown above.

Integrations of 121.6, 1000, 497.9, and 273.1 were observed for peaks C, B, A, and D, respectively.

Hydroboration of Styrene-d_8 (0.3 equiv of BH_3; 22 °C). To 3 mL (3 mmol) of 1 M borane in THF at 22 °C was added 1.04 mL (1.01 g, 9 mmol) of styrene-d_8 by syringe. After stirring 4 h at 22 °C, the mixture was cooled to 0 °C and 1.8 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 20-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 3 mL of ether were added and after 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was removed by rotavap. The resulting solution (~1 mL) was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at δ 4.93, 3.83, 2.94, 1.53 were assigned to positions C, B, A, and D in the 2-pentadeuterophenyl-1,1,2,-trideutero-ethanol and 1-pentadeuteropheny-l-1,2,2-trideutero-ethanol products as shown above. Integrations of 99.0, 1000, 510.5, and 211.5 were observed for peaks C, B, A, and D, respectively.

Hydroboration of Styrene-d_8 (100 equiv of BH_3; 0 °C). To 10 mL (10 mmol) of 1 M borane in THF at 0 °C was added 11.6 μL (11.2 mg, 0.1 mmol) of styrene-d_8 by syringe. After stirring 4 h at 0 °C, the mixture was cooled to -78 °C and 6 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 6 mL of ether were added. After 30 min of stirring, Na_2SO_4

was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 4 mL of ether, then the excess solvent was removed by rotavap. The resulting solution (~1 mL) was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). The ^{2}H NMR peaks at δ 4.93, 3.83, 2.94, 1.53 were assigned to positions C, B, A, and D in the 2-pentadeuterophenyl-1,1,2,-trideutero-ethanol and 1-pentadeuteropheny-l-1,2,2-trideutero-ethanol products as shown above. Integrations of 133.2, 1000, 488.6, and 268.7 were observed for peaks C, B, A, and D, respectively.

Hydroboration of Styrene-d_8 (100 equiv of BH_3; - 28 °C). To 25 mL (25 mmol) of 1 M borane in THF at -28 °C was added 29 μL (28.1 mg, 0.25 mmol) of styrene-d8 by syringe. After stirring ~110 h at -28 °C, a 1-mL aliquot of the resulting solution was then quenched at -28 °C with 1.2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 5-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 2 mL of ether were added and after 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was removed by rotavap. The resulting solution (~1 mL) was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL $CDCl_3$). The ^{2}H NMR peaks at δ 4.93, 3.83, 2.94, 1.53 were assigned to positions C, B, A, and D in the 2-pentadeuterophenyl-1,1,2,-trideutero-ethanol and 1-pentadeuteropheny-l-1,2,2-trideutero-ethanol products, as shown above. Integrations of 98.8, 1000, 510.5, and 229.4 were observed for peaks C, B, A, and D, respectively.

Independent Hydroboration of Styrene-d_8 (100 equiv of BH_3; - 28 °C). To 25 mL (25 mmol) of 1 M borane in THF at -28 °C was added 29 μL (28.1 mg, 0.25 mmol) of styrene-d_8 by syringe. After stirring ~110 h at -28 °C, a 1-mL aliquot of the resulting solution was then quenched at -28 °C with 1.2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 5-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 2 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was removed by rotavap. The resulting solution (~1 mL) was then analyzed directly by ^2H NMR (400 MHz, 5 μL $CDCl_3$). The ^2H NMR peaks at d 4.93, 3.83, 2.94, 1.53 were assigned to positions C, B, A, and D in the 2-pentadeuterophenyl-1,1,2,-trideutero-ethanol and 1-pentadeuteropheny-l-1,2,2-trideutero-ethanol products as shown above. Integrations of 84.5, 1000, 473.0, and 236.5 were observed for peaks C, B, A, and D, respectively.

Stock Solution of 1:1 H:D Borane. A stock solution of 1 M borane in THF containing an approximately equal mixture of hydrogen and deuterium was prepared by mixing 2 mL of 1 M BH_3 in THF with 2 mL of 1 M BD_3 in THF. To allow for the departure of this solution from a precisely 1:1 ratio of H:D, the same stock solution was used to prepare isotopic "standard" (where no isotopic fractionation had occurred) and "sample" (prepared under conditions in which isotopic fractionation occurs).

"Standard" for the Hydroboration of Styrene with 1:1 H:D Borane. To 0.5 mL of the mixture of boranes in THF at 22 °C was added 174 μL (158 mg, 1.52 mmol)

of styrene-d_8 by syringe. After stirring for 30 min at 22 °C, the resulting solution was then quenched with 0.5 mL of 3 M NaOH in water were added dropwise over a 5-min period followed by 0.5 mL of 30% H_2O_2 in water was added dropwise over a 5-min period. The quenched mixture was stirred overnight. The next day, 2 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was removed by rotavap. The product oil was then keep under high vacuum for ~3 h. The final mixture 54 mg was dissolved in ~0.7 mL of $CDCl_3$ and 5 μL of *o*-dichlorobenzene were added as standard. This sample was first analyzed by ^1H NMR (400 MHz, 3 μL pyridine). The integration of CH_2O signal at δ 3.83 was 1346.68. A second spectra gave 1389.53

"Sample" for the Hydroboration of Styrene with 1:1 H:D Borane. To 1.5 mL of the mixture of boranes in THF at 22 °C was added 57 μL (55 mg, 0.5 mmol) of styrene-d_8 by syringe. After stirring for 30 min at 22 °C, the resulting solution was then quenched with 1 mL of 3 M NaOH in water were added dropwise over a 5-min period followed by 1 mL of 30% H_2O_2 in water was added dropwise over a 5-min period. The quenched mixture was stirred overnight. The next day, 2 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was removed by rotavap. The product oil was then keep under high vacuum for ~3 h. The final mixture 143 mg was dissolved in ~0.7 mL of $CDCl_3$ and 5 μL of *o*-

dichlorobenzene were added as standard. This sample was analyzed by ^{1}H NMR (400 MHz, 3 μL pyridine), and the integration of CH_2O signal at d 3.83 was 1348.68.

A second spectra gave 1372.67. The peaks for the benzylic hydrogens at δ 2.84 and δ 1.46 were also intergrated as displayed in Figure **7.1** and Figure **7.2** and listed in Tables **7.1** and **7.2**.

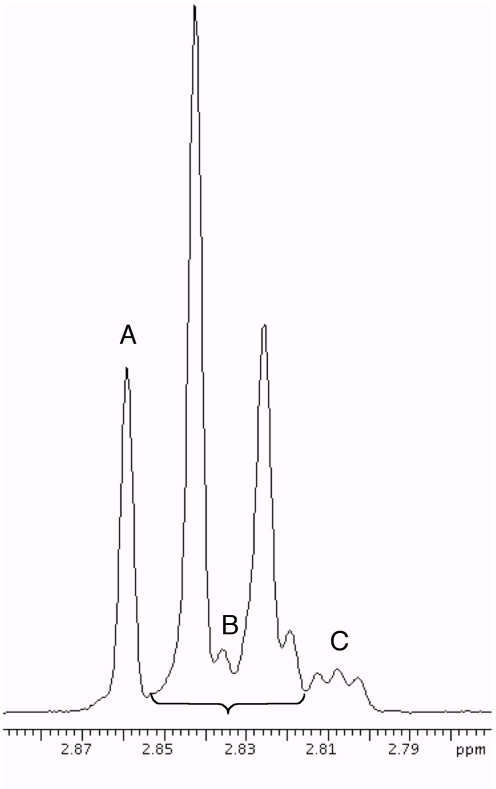


Figure 7.1. Peaks intergrated for the benzylic hydrogens at δ 2.84 displayed above.

Table 7.1. Integrations for the benzylic hydrogens at δ 2.84 displayed above.

	A	B	C
Standard	100	486.8	66.4
Sample	100	495.8	66.2
Standard	100	453.1	62.6
Sample	100	413.7	60.8

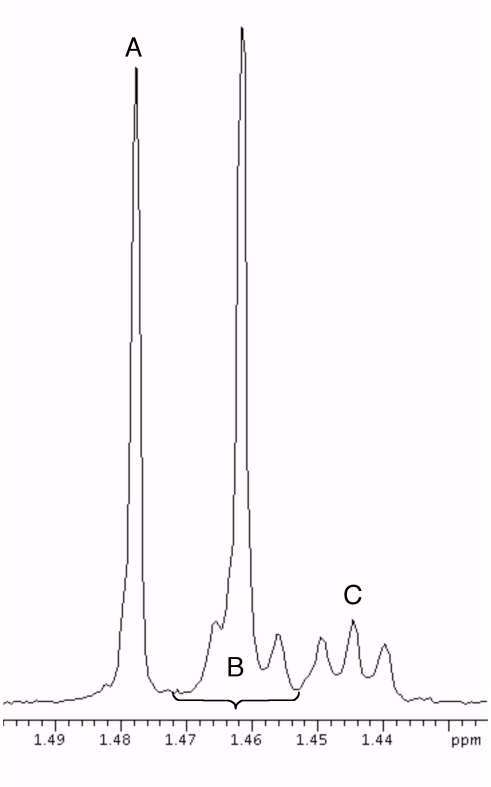


Figure 7.2. Peaks intergrated for the benzylic hydrogens at δ 1.46 displayed above.

Table 7.2. Integrations for the benzylic hydrogens at δ 1.47 displayed above.

	A	C
Standard	100	51.1
Sample	100	52.1

Independent Stock Solution of 1:1 H:D Borane. A stock solution of 1 M borane in THF containing an approximately equal mixture of hydrogen and deuterium was prepared by mixing 2 mL of 1 M BH_3 in THF with 2 mL of 1 M BD_3 in THF. To allow for the departure of this solution from a precisely 1:1 ratio of H:D, the same stock solution was used to prepare isotopic "standard" (where no isotopic fractionation had

occurred) and "sample" (prepared under conditions in which isotopic fractionation occurs).

"Standard" for the Hydroboration of Styrene with 1:1 H:D Borane. To 1.5 mL of the mixture of boranes in THF at 22 °C was added 514 μL (468 mg, 4.5 mmol) of styrene by syringe. After stirring for 30 min at 22 °C, the resulting solution was then quenched with 0.5 mL of 3 M NaOH in water were added dropwise over a 5-min period followed by 0.5 mL of 30% H_2O_2 in water was added dropwise over a 5-min period. The quenched mixture was stirred overnight. The next day, 2 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was evaporated. The final mixture 473 mg was dissolved in ~0.7 mL of $CDCl_3$ and 5 μL of *o*-dichlorobenzene were added as standard. This sample was analyzed by ^1H NMR (400 MHz, 3 μL pyridine). The integration of CH_2O signal at d 3.83 was 1633.69.

"Sample" for the Hydroboration of Styrene with 1:1 H:D Borane. To 1.5 mL of the mixture of boranes in THF at 22 °C was added 57 μL (52 mg, 0.5 mmol) of styrene by syringe. After stirring for 30 min at 22 °C, the resulting solution was then quenched with 1 mL of 3 M NaOH in water were added dropwise over a 5-min period followed by 1 mL of 30% H_2O_2 in water was added dropwise over a 5-min period. The quenched mixture was stirred overnight. The next day, 2 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess

solvent was evaporated. The final mixture 534 mg was dissolved in ~0.7 mL of $CDCl_3$ and 3 μL pyridine were added as standard. This sample was analyzed by ^1H NMR (400 MHz, 3 μL pyridine). The integration of CH_2O signal at δ 3.83 was 1374.88 (Tables **7.3** and **7.4**).

Table 7.3. Integrations for the benzylic hydrogens at δ 2.84 displayed above.

	A	B	C
Standard	100	409	40.7
Sample	100	425.6	39.5

Table 7.4. Integrations for the benzylic hydrogens at δ 1.46 displayed above.

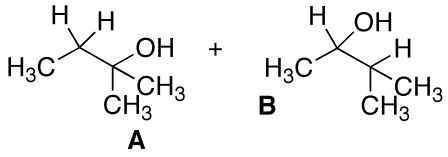
	A	B
Standard	100	49.2

Experimental Procedures for 'Hydroboration of Internal Disubstituted and Trisubstituted Alkenes

Hydroboration of 2-methyl-2-butene (100 equiv of BH_3). To 18 mL (187 mmol) of borane dimethyl sulfide complex at 22 °C was added 0.2 mL (132 mg, 1.9 mmol) of 2-methyl-2-butene by syringe. After stirring ~12 h at 22 °C, the solution was then quenched with 150 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water at 0 °C. The reaction mixture was added dropwise over a 6 h period to the water solution. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 5 mL of toluene-d_8 were added. After 30 min of stirring, the 5 mL mixture of toluene-d_8 was extracted. Dried over Na_2SO_4 and filtered using 2 mL of

toluene-d_8. The resulting sample was then analyzed by ^{1}H NMR (500 MHz, toluene-d_8). The integrations corresponding to 2-methyl-2-butanol and 3-methyl-2-butanol were 19.8 and 274.3 observed for peaks A, and B, shown in the picture below, respectively.

Scheme 7.7



Hydroboration of 2-methyl-2-butene (0.7 equiv of BH_3). To 0.3 mL (3.0 mmol) of borane dimethyl sulfide complex at 22 °C was added 0.42 mL (277 mg, 4.1 mmol) of 2-methyl-2-butene by syringe. After stirring ~12 h at 22 °C, the resulting solution was then quenched at 0 °C with 4 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 60-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 2 mL of toluene-d_8 were added. After 30 min of stirring, the 2 mL mixture of toluene-d_8 was extracted. Dried over Na_2SO_4 and filtered using 2 mL of toluene-d_8. The resulting sample was then analyzed by ^{1}H NMR (500 MHz, toluene-d_8). The integrations corresponding to 2-methyl-2-butanol and 3-methyl-2-butanol were 3.8 and 100 observed for peaks A, and B, shown in the picture below, respectively.

Hydroboration of 3-methylcyclohexene (0.7 equiv of BH_3). To 1.0 mL (790 mg, 10.4 mmol) of borane dimethyl sulfide complex at 22 °C was added 1.7 mL (1.4 g, 14.8 mmol) of 3-methylcyclohexene by syringe. After stirring ~12 h at 22 °C, the

solution was then quenched at 0 °C with 6 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 2 h period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 2 mL of toluene-d_8 were added. After 30 min of stirring, the 2 mL mixture of toluene-d_8 was extracted. Dried over Na_2SO_4 and filtered using 2 mL of toluene-d_8. The resulting sample was then analyzed by ^{1}H NMR (500 MHz, toluene-d_8). The integrations corresponding to the products are shown in the picture below and are displayed in Table **7.5**.

Scheme 7.9

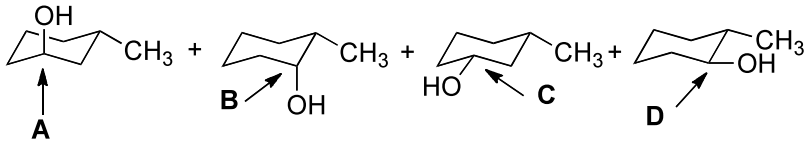


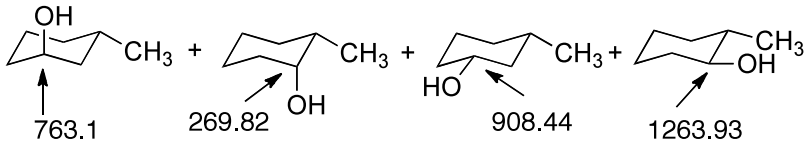
Table 7.5. Integrations for the hydrogen on the carbon indicated by the arrow in Scheme 7.9 for each product.

	A	B	C	D
Integration	1000	473.4	1131.42	1139.85
% Ratio	26.7	12.64	30.21	30.44

Hydroboration of 3-methylcyclohexene (44 equiv of BH_3). To 8.75 mL (6.9 g, 91 mmol) of borane dimethyl sulfide complex at 22 °C was added 0.26 mL (9.96 g, 104 mmol) of 3-methylcyclohexene by syringe. After stirring ~12 h at 22 °C, the solution was then quenched with 100 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water at 0 °C. The reaction mixture was added dropwise over a 6-8 h period to the

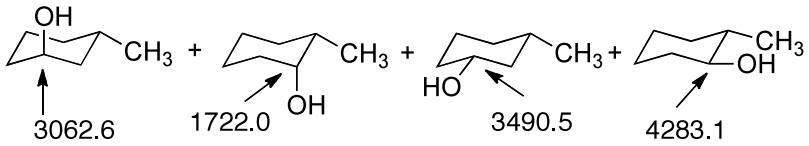
water solution. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 5 mL of toluene-d_8 were added. After 30 min of stirring, the 5 mL mixture of toluene-d_8 was extracted. Dried over Na_2SO_4 and filtered using 2 mL of toluene-d_8. The resulting sample was then analyzed by ^1H NMR (500 MHz, toluene-d_8). The integrations corresponding to the products are shown in the picture below.

Scheme 7.10



Hydroboration of 3-methylcyclohexene (100 equiv of BH_3). To 20.1 mL (15.9 g, 209 mmol) of borane dimethyl sulfide complex at 22 °C was added 0.26 mL (209 mg, 2.1 mmol) of 3-methylcyclohexene by syringe. After stirring ~12 h at 22 °C, the solution was then quenched with 200 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water at 0 °C. The reaction mixture was added dropwise over a 6 h period to the water solution. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. To the mixture, 10 mL of toluene-d_8 were added. After 30 min of stirring, the 10 mL mixture of toluene-d_8 was extracted. Dried over Na_2SO_4 and filtered using 3 mL of toluene-d_8. The resulting sample was then analyzed by ^1H NMR (500 MHz, toluene-d_8). The integrations corresponding to the products are shown in the picture below.

Scheme 7.11



Stock Solution of 30:70 H:D Borane. The stock solution of 1 M borane in THF was prepared by mixing 9 mL of 1 M BH_3 in THF with 21 mL of 1 M BD_3 in THF.

"Standard" for the Hydroboration of 2-Methyl-2-Butene and Tetramethylethylene with 30:70 H:D Borane. To determine the actual ratio of H to D in the 30:70 stock solution, 1.0 mL (1 mmol) of the solution was reacted with 0.47 mL (337 mg, 3 mmol) of 1-octene for 30 min at 22 °C, the resulting solution was then quenched with 0.5 mL of 3 M NaOH in water were added dropwise over a 5-min period followed by 0.5 mL of 30% H_2O_2in water was added dropwise over a 5-min period. The quenched mixture was stirred overnight. The next day, 1 mL of ether was added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min, the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was evaporated. The resulting 1-octanol was analyzed by ^{13}C NMR under integration-appropriate conditions,[48] and the ratio of the deuterated versus non-deuterated 1-octanol product by integration of the resolved ^{13}C NMR signals of the two materials (intergrations are displayed in Table **7.6**).

Table 7.6. Integrations of the resolved ^{13}C NMR signals for deuterated and non-deuterated products.

δ 32.48	δ 32.26	δ 32.07	δ 31.88
H	D	D	D
100	69.31	67.9	71.1

100	65.66	65.28	67.49
148.45	96.55	94.81	96.98
100	69	64	64

"Sample 1" for the Hydroborations of 2-Methyl-2-Butene with 30:70 H:D Borane. The hydroboration of 2-methyl-2-butene was carried out by the dropwise addition of 0.25 mL (166 mg, 2.36 mmol) of 2-methyl-2-butene to 7.1 mL (7.1 mmol) of the stock borane solution and stirring for 12 h at 22 °C, the resulting solution was then quenched with 5 mL of 3 M NaOH in water were added dropwise over a 25-min period followed by 5 mL of 30% H_2O_2 in water was added dropwise over a 25-min period. The quenched mixture was stirred overnight. The next day, 5 mL of ether were added. After 30 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was evaporated. The resulting crude 3-methyl-2-butanol was analyzed by ^1H NMR in $CDCl_3$. The doublet at ~δ 1.1 ppm was 925.6 and the multiplet at ~δ 0.8 ppm was 1906.0.

"Sample 2" for the Hydroborations of 2-Methyl-2-Butene with 30:70 H:D Borane. The hydroboration of 2-methyl-2-butene was carried out by the dropwise addition of 0.25 mL (166 mg, 2.36 mmol) of 2-methyl-2-butene to 0.75 mL (0.75 mmol) of the stock borane solution and stirring for 30 min at 22 °C, the resulting solution was then quenched with 0.5 mL of 3 M NaOH in water were added dropwise over a 5-min period followed by 0.5 mL of 30% H_2O_2 in water was added dropwise over a 5-min

period. The quenched mixture was stirred overnight. The next day, 1 mL of ether was added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 1 mL of ether, then the excess solvent was evaporated. The resulting crude 3-methyl-2-butanol was analyzed by ^1H NMR in $CDCl_3$. The doublet at ~δ 1.1 ppm was 964.7 and the multiplet at ~δ 0.8 ppm was 1960.7.

"Sample 3" for the Hydroborations of 2-Methyl-2-Butene with 30:70 H:D Borane. The hydroboration of 2-methyl-2-butene was carried out by the dropwise addition of 0.25 mL (166 mg, 2.36 mmol) of 2-methyl-2-butene to 0.75 mL (0.75 mmol) of the stock borane solution and stirring for 30 min at 22 °C, the resulting solution was then quenched with 0.6 mL of 3 M NaOH in water were added dropwise over a 5-min period followed by 0.6 mL of 30% H_2O_2in water was added dropwise over a 5-min period. The quenched mixture was stirred overnight. The next day, 1 mL of ether was added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 1 mL of ether, then the excess solvent was evaporated. The resulting crude 3-methyl-2-butanol was analyzed by ^1H NMR in $CDCl_3$. The doublet at ~δ 1.1 ppm was 918.8 and the multiplet at ~δ 0.8 ppm was 1907.4.

"Sample" for the Hydroborations of Tetramethylethylene with 30:70 H:D Borane. The hydroboration of tetramethylethylene was carried out by the dropwise addition of 0.24 mL (168 mg, 2.0 mmol) of 2,3-dimethyl-2-butene to 2 mL (2 mmol) of the stock borane solution and stirring for 30 min at 22 °C, the resulting solution was then

quenched with 1.5 mL of 3 M NaOH in water were added dropwise over a 10-min period followed by 1.5 mL of 30% H_2O_2 in water was added dropwise over a 10-min period. The quenched mixture was stirred overnight. The next day, 2 mL of ether were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was evaporated. The resulting crude 2,3-dimethyl-2-butanol was analyzed by ^1H and ^{13}C NMR in $CDCl_3$. The integrations for ^1H NMR are 200 and 315.0. A different spectrum gave 200 and 320.2. The ^{13}C NMR under integration-appropriate conditions,[48] integrated to 200 and 317.5 for the non-deuterated and deuterated products respectively.

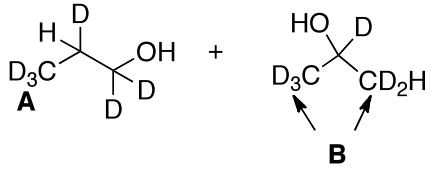
"Sample 2" for the Hydroborations of tetramethylethylene with 30:70 H:D Borane.The hydroboration of tetramethylethylene was carried out by the dropwise addition of 0.24 mL (168 mg, 2.0 mmol) of 2,3-dimethyl-2-butene to 2 mL (2 mmol) of the stock borane solution and stirring for 30 min at 22 °C, the resulting solution was then quenched with 1.5 mL of 3 M NaOH in water were added dropwise over a 10-min period followed by 1.5 mL of 30% H_2O_2in water was added dropwise over a 10-min period. The quenched mixture was stirred overnight. The next day, 2 mL of ether were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. After 30 more min the ether solution was filtered and rinsed using 2 mL of ether, then the excess solvent was evaporated. The resulting crude 2,3-dimethyl-2-butanol was analyzed by ^1H and ^{13}C NMR in $CDCl_3$. The integrations for ^1H NMR are 200 and

327.3. The ^{13}C NMR under integration-appropriate conditions,[48] integrated to 200 and 324.1 for the non-deuterated and deuterated products respectively.

Experimental Procedures for 'Dynamics and Selectvitity in the Hydroboration of Alkenes *via* Chloroboranes

Hydroboration of Propene-d_6 with $BH_2Cl{\bullet}SMe_2$ Neat (22 °C, 1.5 equiv of borane). To 0.11 mL (114 mg, 4.05 mmol) of monochloroborane dimethyl sulfide complex at 22 °C was added 0.1 mL (52 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 12 h at 22 °C, the mixture was cooled to 0 °C and 4 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis, 2 mL of water and 1 mL of methanol were added. A 1-mL aliquot of the solution was then analyzed directly by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 49.27 were observed for peaks A and B, respectively.

Scheme 7.12



Hydroboration of Propene-d_6 with $BH_2Cl{\bullet}SMe_2$ Neat (3 °C, 1.5 equiv of borane). To 0.11 mL (114 mg, 4.05 mmol) of monochloroborane dimethyl sulfide complex at 3 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -

48 °C) by cannula. After stirring 5 h at 3 °C, the mixture was quenched with 4 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample, water and methanol were added. A 1-mL aliquot of the solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 45.41 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with BH_2Cl•SMe_2 Neat (45 °C, 1.5 equiv of borane). To 0.11 mL (114 mg, 4.05 mmol) of monochloroborane dimethyl sulfide complex at 45 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 5 h at 45 °C, the mixture was cooled to 0 °C and with 4 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample, water and methanol were added. A 1-mL aliquot of the solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 51.57 were observed for peaks A and B, respectively.

Hydroboration of Propene-d6 with BH_2Cl•SMe_2 Neat (60 °C, 1.5 equiv of borane). To 0.11 mL (114 mg, 4.05 mmol) of monochloroborane dimethyl sulfide complex at 60 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 5 h at 60 °C, the mixture was cooled to 0 °C and with 4 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise

over a 30-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample, water and methanol were added. A 1-mL aliquot of the solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 60.09 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with BH_2Cl•dioxane (22 °C, 1.5 equiv of borane). To 1.62 mL (4.05 mmol) of monochloroborane dioxane complex (2.5 M in dichloromethane) at 22 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 15 h at 22 °C, the mixture was cooled to 0 °C and with 2.5 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 20-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 46.6 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with BH_2Cl•dioxane (3 °C, 1.5 equiv of borane). To 1.62 mL (4.05 mmol) of monochloroborane dioxane complex (2.5 M in dichloromethane) at 3 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 8 h at 3 °C, the mixture was cooled to 0 °C and with 2.5 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was

added dropwise over a 30-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 2441.8 and 85.19 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with BH_2Cl•dioxane (45 °C, 1.5 equiv of borane). To 1.62 mL (4.05 mmol) of monochloroborane dioxane complex (2.5 M in dichloromethane) at 45 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 30-min at 45 °C, the mixture was cooled to 0 °C and with 2.5 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 21 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 59.49 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with BH_2Cl•dioxane (60 °C, 1.5 equiv of borane). To 1.62 mL (4.05 mmol) of monochloroborane dioxane complex (2.5 M in dichloromethane) at 60 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed

propene-d_6 (at -48 °C) by cannula. After stirring 30-min at 60 °C, the mixture was cooled to 0 °C and with 2.5 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 20-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 137.79 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with BH_2Cl•dioxane (3 °C, 2 equiv of borane). To 0.72 mL (1.8 mmol) of monochloroborane dioxane complex (2.5 M in dichloromethane) at 3 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d6 (at -48 °C) by cannula. After stirring 8 h at 3 °C, the mixture was cooled to 0 °C and with 1.1 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 45.1 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•SMe_2 Neat (3 °C, 1 equiv of borane). To 0.31 mL (389 mg, 2.7 mmol) of dichloroborane dimethyl sulfide complex at 3 °C was added 0.1 mL (52 mg, 2.7 mmol) of condensed propene-d6 (at -48 °C) by cannula. After stirring for 12 h at 3 °C, the mixture quenched with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 20-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis, 2 mL of water were added. A 1-mL aliquot of the solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 527.4 and 21.8 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•SMe_2 Neat (22 °C, 2 equiv of borane). To 0.62 mL (778 mg, 5.4 mmol) of dichloroborane dimethyl sulfide complex at 22 °C was added 0.1 mL (52 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 12 h at 22 °C, the mixture was cooled to 0 °C and 4 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 40-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis, ~2 mL of water were added. A 1-mL aliquot of the solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1863 and 90.2 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•SMe_2 Neat (3 °C, 2 equiv of borane). To 0.62 mL (778 mg, 5.4 mmol) of dichloroborane dimethyl sulfide complex at

3 °C was added 0.1 mL (52 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 12 h at 3 °C, the mixture was cooled to 0 °C and 4 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 40-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis, ~2 mL of water were added. A 1-mL aliquot of the solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 867.4 and 31.0 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•SMe_2 Neat (60 °C, 2 equiv of borane). To 0.62 mL (778 mg, 5.4 mmol) of dichloroborane dimethyl sulfide complex at 60 °C was added 0.1 mL (52 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 12 h at 60 °C, the mixture was cooled to 0 °C and 4 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 40-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis, ~2 mL of water were added. A 1-mL aliquot of the solution was then analyzed directly by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1283 and 73.2 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•dioxane (22 °C, 1 equiv of borane). To 0.9 mL (2.7 mmol) of dichloroborane dioxane complex (2.5 M in dichloromethane) at 22 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 15 h at 22 °C, the mixture was cooled to 0 °C and with 2 mL of a

1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 40.2 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•dioxane (3 °C, 1 equiv of borane). To 0.9 mL (2.7 mmol) of dichloroborane dioxane complex (2.5 M in dichloromethane) at 3 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 8 h at 3 °C, the mixture was quenched with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 43.2 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•dioxane (45 °C, 1 equiv of borane). To 0.9 mL (2.7 mmol) of dichloroborane dioxane complex (2.5 M in dichloromethane)

at 45 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 1 h at 45 °C, the mixture was cooled to 0 °C and with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 37.3 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•dioxane (60 °C, 1 equiv of borane). To 0.9 mL (2.7 mmol) of dichloroborane dioxane complex (2.5 M in dichloromethane) at 60 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 1 h at 60 °C, the mixture was cooled to 0 °C and with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^{2}H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1000 and 43.9 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•dioxane (22 °C, 2.5 equiv of borane). To 2.2 mL (6.7 mmol) of dichloroborane dioxane complex (2.5 M in dichloromethane) at 22 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 15 h at 22 °C, the mixture was cooled to 0 °C and with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 823.64 and 40.2 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•dioxane (3 °C, 2.5 equiv of borane). To 2.2 mL (6.7 mmol) of dichloroborane dioxane complex (2.5 M in dichloromethane) at 3 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring 8 h at 3 °C, the mixture was quenched with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400

MHz, 5 μL pyridine-d_6). Integrations of 11081.3 and 516 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$•dioxane (45 °C, 2.5 equiv of borane). To 2.2 mL (6.7 mmol) of dichloroborane dioxane complex (2.5 M in dichloromethane) at 45 °C was added 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 1 hstirring for 1 h at 45 °C, the mixture was cooled to 0 °C and with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2 mL of $CHCl_3$ were added. After 10 min of stirring, Na_2SO_4 was added slowly to remove the aqueous layer. A 1-mL aliquot of the solution was flittered though a pipette with cotton into the NMR tube for direct analysis by ^2H NMR (400 MHz, 5 μL pyridine-d_6). Integrations of 1114.34 and 60.94 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with BH_2Cl (22 °C, 0.5 equiv of BCl_3). To 0.12 mL (164 mg 1.4 mmol) of condensed BCl_3 (at -78 °C) was added 0.45 mL (326 mg, 1.4 mmol) of diethylsilane. The solution was allowed to warm to 22 °C and 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 12 h at 22 °C, the mixture was cooled to 0 °C and with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 2

mL of THF and 2 mL of methanol were added. A 1-mL aliquot of the solution was analyzed directly by ^{2}H NMR (400 MHz, 3 μL $CDCl_3$). Integrations of 1000 and 23.1 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with BH_2Cl (22 °C, excess of BCl_3). To 1.2 mL (1.64 g 14 mmol) of condensed BCl_3 (at -78 °C) was added 4.5 mL (3.26 g, 14 mmol) of diethylsilane. The solution was allowed to warm to 22 °C and 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) by cannula. After stirring for 12 h at 22 °C, the mixture was cooled to 0 °C and with 10 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 10 mL of THF and 13 mL of methanol were added. A 1-mL aliquot of the solution was analyzed directly by ^{2}H NMR (400 MHz, 3 μL $CDCl_3$). Integrations of 1000 and 23.1 were observed for peaks A and B, respectively.

Hydroboration of Propene-d_6 with $BHCl_2$ (22 °C, 1 equiv of BCl_3). To 0.125 mL (166 mg 1.4 mmol) of condensed BCl_3 (at -78 °C) was added 0.224 mL (163 mg, 1.4 mmol) of triethylsilane. The solution was allowed to warm to 22 °C and 0.1 mL (65 mg, 1.4 mmol) of condensed propene-d_6 (at -78 °C) was added by cannula. After stirring for 12 h at 22 °C, the mixture was cooled to 0 °C and with 2 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 10-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous

sample 2 mL of THF and 2 mL of methanol were added. A 1-mL aliquot of the solution was analyzed directly by ^{2}H NMR (400 MHz, 3 μL $CDCl_3$). The Markovnikov product was not detected.

Hydroboration of Propene-d_6 with $BHCl_2$ (22 °C, excess of BCl_3). To 1.25 mL (1.66 g 14 mmol) of condensed BCl_3 (at -78 °C) was added 2.24 mL (1.63 g, 14 mmol) of triethylsilane. The solution was allowed to warm to 22 °C and 0.25 mL (130 mg, 2.7 mmol) of condensed propene-d_6 (at -48 °C) was added by cannula. After stirring for 12 h at 22 °C, the mixture was cooled to 0 °C and with 10 mL of a 1:1 mixture of 3 M NaOH in water and 30% H_2O_2 in water was added dropwise over a 30-min period. The resulting mixture was allowed to warm to 22 °C and was stirred overnight. The quenched reaction separated into two layers. To allow direct analysis of a homogeneous sample 10 mL of THF and 10 mL of methanol were added. A 1-mL aliquot of the solution was analyzed directly by ^{2}H NMR (400 MHz, 3 μL $CDCl_3$). Integrations of 1000 and 13.4 were observed for peaks A and B, respectively.

CHAPTER VIII

SUMMARY AND CONCLUSIONS

Transition state theory is the foundation that chemists rely on to explain reactivity and selectivity. Within transition state theory, the rate of product formation is related to the energy of the transition state. The favored product is determined by the transition state with the lowest energy. The product selectivity is determined by the difference in energy for the different transition states. The mechanism of a reaction is explained as a series of transition states and intermediates leading to the product.

It is found here that transition state theory fails in an example where it is ubiquitously invoked, the hydroboration of alkenes with BH_3. High-level *ab initio* calculations predict too large of an energy difference between competitive transition structures to account for the observed product ratio, and the consideration of calculational error, solvent, tunneling, and entropy effects does not resolve the discrepancy. Trajectory studies, however, predict well the experimental selectivity. This means that in this most 'textbook' of reactions, transition state theory fails and the selectivity can only be understood by consideration of dynamic trajectories.

In the case of the hydroboration of styrene, transition state theory was used to explain experimental selectivity. We found that this was not the appropriate method to accurately predict regioselectivity hydroboration reactions. G3B3 calculations predict too large of an energy difference between competitive transition structures to account for the experimentally observed product ratio. Considering calculational errors, tunneling, and entropy effects does not account for the discrepancy. However, trajectories started

from the enthalpic association barrier found following the steepest-descent path, better predict the experimental selectivity. This represents another example in which transition state theory is proven to be inapplicable when the branching deciding the selectivity located after the rate-limiting transition structure. In this well-know reaction, consideration of dynamic trajectories is essential for explaining the experimental outcome.

The hydroboration of internal disubstituted and trisubstituted alkenes showed that an entropic association barrier for the formation of π-complex was present in all cases. It was determined for the internal disubstituted and trisubstituted alkenes that the formation of such π-complex is enthalpically barrierless. Dynamics cases were established, when the enthalpic association barrier found was the rate-limiting step and the barrier for the formation of products from π-complex were small. Various isotope effects were determined. The isotope effects for the hydroboration of propene, tetramethylethylene, styrene, and 2-methyl-2-butene with BH_3/BD_3 mixture were determined. These isotope effects were too small for the conventional mechanism to be the predominate pathway.

When the hydroboration reaction of propene with BH_2Cl or $BHCl_2$ was explored through a series of experimental and theoretical studies, we observed that the regioselectivity was lower than can be accounted for by transition state theory. The calculated pathways indicated that energy barriers were too large for the complexes to overcome to be considered a "hot" reaction. The regioselectivity discrepancy was attributed to the chloroboranes undergoing equilibrium with the starting material. A

more crucial piece of information that fits here is the observation by Brown for $(ClCH_2CH_2)_2O{\cdot}BHCl_2$ in dichloromethane. Using this reagent with a variety of olefins he was able to measure the amount of BCl_3 generated by ^{11}B NMR. At room temperature, an 8% of BCl_3 was generated from the reaction of 1-octene with dichloroborane. The amount of R_2BCl generated was 2%, relative to the amount of $RBCl_2$. For the reaction with other alkenes like cyclohexene, 50% of BCl_3 and 28% of R_2BCl were detected.

From the theoretical paths calculated for representative cases for the hydroboration of chloro and ethoxy functional derivative alkenes, we found an entropic association barrier for the formation of π-complex in all cases. It was determined for allylchloride and ethoxy functional alkenes that the formation of such π-complexes is enthalpically barrierless. Dynamics cases were establish, when the enthalpic association barrier found was the rate-limiting step and the barrier for the formation of products from the π-complex was small. For chlorocyclohexene, the results were inconclusive. Whereas in the case of the hydroboration of methoxycyclohexene with BH_3, just like in the case of 2-methyl-2-butene, we suggested an accidental agreement of transition state theory with experiment

In some cases TST may not be an appropriate method to use for modeling reaction reactivity and selectivity. Other theories such as, dynamic effects, have proven to be more acceptable computational models to follow due to its inclusion of entropic barriers. Transition state theory is a model for reactivity that can fail. The origin of this term is that when transition state theory fails, one must fall back on the detailed

consideration of the motions and momenta of atoms. The consideration of dynamic effects is essential for the understanding of the mechanism in a diversity of reactions.

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APPENDIX

DETAILED COMPUTATIONAL INFORMATION

A. 1. Theoretical Structures from "Dynamics and the Failure of Transition State Theory in the Hydroboration of Terminal Alkenes with BH_3"

2a-1‡ Transition State

B3LYP/6-31G*

E(RB+HF-LYP) = -144.539006748

Zero-point correction= 0.112473
Thermal correction to Energy= 0.117645
Thermal correction to Enthalpy= 0.118589
Thermal correction to Gibbs Free Energy= 0.085451
Sum of electronic and ZPE= -144.426533
Sum of electronic and thermal Energies= -144.421362
Sum of electronic and thermal Enthalpies= -144.420418
Sum of electronic and thermal Free Energies= -144.453556

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.823	18.753	69.744

C,0,0.0103882876,0.0256028808,0.0056736821
C,0,-0.0158768703,0.0164285883,1.5129040978
C,0,1.1494814125,0.0161014193,2.2898767973
B,0,0.4646825308,1.6346562743,2.3350624949
H,0,-0.8920054427,0.4748855541,-0.4191447445
H,0,0.0790220168,-1.0097071762,-0.3523925903
H,0,-0.9346989994,-0.3403132133,1.9728457627
H,0,2.1143205352,0.0308742072,1.7927199234
H,0,1.1362782935,-0.4218047415,3.2814035473
H,0,0.149460483,1.825180382,3.4754349653
H,0,-0.5970626953,1.6955092492,1.7089844612
H,0,1.2260979562,2.3369179467,1.7309522008
H,0,0.882188492,0.5719806289,-0.3662085979

MP4/cc-pvdz

MP4SDTQ=-144.0826608

Zero-point correction= 0.111781
Thermal correction to Energy= 0.117048
Thermal correction to Enthalpy= 0.117992

Thermal correction to Gibbs Free Energy= 0.084666
Sum of electronic and ZPE= -143.970880
Sum of electronic and thermal Energies= -143.965613
Sum of electronic and thermal Enthalpies= -143.964668
Sum of electronic and thermal Free Energies= -143.997995

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.449	19.134	70.142

C
C,1,cc2
C,2,cc3,1,ccc3
B,3,bc4,2,bcc4,1,dih4,0
H,1,hc5,2,hcc5,3,dih5,0
H,1,hc6,2,hcc6,3,dih6,0
H,2,hc7,3,hcc7,4,dih7,0
H,3,hc8,2,hcc8,1,dih8,0
H,3,hc9,2,hcc9,1,dih9,0
H,4,hb10,2,hbc10,1,dih10,0
H,4,hb11,2,hbc11,1,dih11,0
H,4,hb12,2,hbc12,1,dih12,0
H,1,hc13,2,hcc13,3,dih13,0
Variables:
cc2=1.51374033
cc3=1.40481134
ccc3=122.29412762
bc4=1.80948646
bcc4=70.87808166
dih4=102.5351228
hc5=1.1035294
hcc5=111.76583187
dih5=-153.02155639
hc6=1.10685241
hcc6=108.68761585
dih6=87.06291044
hc7=1.09855252
hcc7=117.97296355
dih7=-96.61607606
hc8=1.09504662
hcc8=119.20991145
dih8=1.72917827
hc9=1.09328772
hcc9=120.11194292

dih9=-156.96633661
hb10=1.21140821
hbc10=118.62039593
dih10=164.19297978
hb11=1.24109322
hbc11=68.23682517
dih11=66.47779814
hb12=1.21254302
hbc12=115.62240298
dih12=-32.74394328
hc13=1.10446572
hcc13=110.28999921
dih13=-31.73498537

CCSD(T)/aug-cc-pvdz

CCSD(T)= -0.14411080571E+03

C
C 1 1.517291
C 2 1.411515 1 121.876
B 3 1.794172 2 71.080 1 102.702 0
H 1 1.103066 2 111.743 3 -153.341 0
H 1 1.106246 2 108.642 3 86.722 0
H 2 1.096999 3 118.172 4 -97.374 0
H 3 1.094314 2 118.882 1 0.936 0
H 3 1.092462 2 119.942 1 -155.853 0
H 4 1.209332 2 118.849 1 162.757 0
H 4 1.246295 2 65.801 1 67.184 0
H 4 1.210882 2 115.636 1 -30.020 0
H 1 1.103830 2 110.189 3 -32.048 0

CBS-QB3

C,0,0.0130871198,0.0234237506,0.0062233583
C,0,-0.0107596956,0.0064780961,1.5105220869
C,0,1.1479128034,0.0073599299,2.284933212
B,0,0.452747201,1.6386467948,2.3300158441
H,0,-0.8867025902,0.4767216712,-0.4128674129
H,0,0.0755353813,-1.0087470141,-0.3550005851
H,0,-0.9298157037,-0.3402028805,1.9709779206
H,0,2.1123644167,0.0390342169,1.7942809699
H,0,1.1334598204,-0.41200007,3.2809728803
H,0,0.1603391539,1.81807887,3.4740593899

H,0,-0.6064912318,1.7134671929,1.7145816819
H,0,1.2259123628,2.3287378571,1.7347221932
H,0,0.8846869619,0.5653135847,-0.365309539

E(ZPE)= 0.110119
E(SCF)= -143.500505
DE(CBS)= -0.062393
DE(CCSD)= -0.019833
DE(Empirical)= -0.034526
CBS-QB3 (0 K)= -144.183859
CBS-QB3 Enthalpy= -144.177636
E(Thermal)= 0.115398
DE(MP2)= -0.645942
DE(MP34)= -0.053962
DE(Int)= 0.023183

CBS-QB3 Energy= -144.178580
CBS-QB3 Free Energy= -144.210957

G3B3

[For the structure, see the B3LYP/6-31G* structure.)

E(ZPE)= 0.107977	E(Thermal)= 0.113305
E(QCISD(T))= -144.010975	E(Empiric)= -0.081120
DE(Plus)= -0.007686	DE(2DF)= -0.158655
E(Delta-G3)= -0.217665	E(G3-Empiric)= -0.081120
G3(0 K)= -144.368125	G3 Energy= -144.362796
G3 Enthalpy= -144.361852	G3 Free Energy=-144.395245

2a-2‡ Transition State

B3LYP/6-31G*

E(RB+HF-LYP) = -144.535327709

Zero-point correction= 0.112552
Thermal correction to Energy= 0.117703
Thermal correction to Enthalpy= 0.118647
Thermal correction to Gibbs Free Energy= 0.085576
Sum of electronic and ZPE= -144.422776
Sum of electronic and thermal Energies= -144.417625
Sum of electronic and thermal Enthalpies= -144.416681
Sum of electronic and thermal Free Energies= -144.449752

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.860	18.647	69.605

H,0,0.0045547581,0.1376409495,0.0281345949
C,0,0.0127679903,0.0727328886,1.1132289927
C,0,1.2342708944,0.0738063991,1.8139082488
B,0,0.4874914161,1.6474426731,1.9179384251
H,0,-0.8868758812,-0.341641882,1.5577716522
C,0,2.5712612723,0.030916587,1.1014769988
H,0,1.2203362285,-0.3723883211,2.8049068149
H,0,0.140520756,1.8160654794,3.0505245842
H,0,-0.5724646284,1.6666766554,1.2647022759
H,0,1.1977745163,2.4000913116,1.317203364
H,0,3.3412536299,0.5575813145,1.6739568737
H,0,2.9050160461,-1.0064018259,0.9644325685
H,0,2.5100060018,0.5020287708,0.1150406066

MP4/cc-pvdz

MP4SDTQ=-144.0791881

Zero-point correction= 0.111890
Thermal correction to Energy= 0.117089
Thermal correction to Enthalpy= 0.118033
Thermal correction to Gibbs Free Energy= 0.084869
Sum of electronic and ZPE= -143.967298
Sum of electronic and thermal Energies= -143.962099
Sum of electronic and thermal Enthalpies= -143.961155
Sum of electronic and thermal Free Energies= -143.994319

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.475	18.922	69.800

H
C,1,ch2
C,2,cc3,1,cch3
B,3,bc4,2,bcc4,1,dih4,0
H,2,hc5,3,hcc5,4,dih5,0
C,3,cc6,2,ccc6,4,dih6,0
H,3,hc7,2,hcc7,4,dih7,0

H,4,hb8,2,hbc8,3,dih8,0
H,4,hb9,2,hbc9,3,dih9,0
H,4,hb10,2,hbc10,3,dih10,0
H,6,hc11,3,hcc11,2,dih11,0
H,6,hc12,3,hcc12,2,dih12,0
H,6,hc13,3,hcc13,2,dih13,0
Variables:
ch2=1.09758041
cc3=1.41512677
cch3=120.02255671
bc4=1.78035513
bcc4=69.43294902
dih4=101.59316564
hc5=1.09588983
hcc5=120.87547848
dih5=-98.65864111
cc6=1.51929769
ccc6=121.88715353
dih6=-106.50504207
hc7=1.09678119
hcc7=116.5161989
dih7=99.26609301
hb8=1.20939085
hbc8=116.87545213
dih8=-87.04302808
hb9=1.25445669
hbc9=65.05338178
dih9=176.95615349
hb10=1.20949965
hbc10=118.03887725
dih10=82.63330935
hc11=1.10434418
hcc11=111.11643048
dih11=147.07619954
hc12=1.10764293
hcc12=110.32916137
dih12=-92.93728276
hc13=1.10513474
hcc13=110.68198966
dih13=27.13340398

CCSD(T)/aug-cc-pvdz

CCSD(T)= -0.14410670939E+03

H
C 1 1.096499
C 2 1.419068 1 119.984
B 3 1.774662 2 69.792 1 101.776 0
H 2 1.094688 3 120.910 4 -98.821 0
C 3 1.523561 2 121.522 4 -106.623 0
H 3 1.095516 2 116.595 4 99.812 0
H 4 1.207805 2 116.761 3 -87.916 0
H 4 1.257629 2 63.950 3 177.070 0
H 4 1.208018 2 117.981 3 83.520 0
H 6 1.103913 3 111.014 2 147.308 0
H 6 1.107039 3 110.524 2 -92.565 0
H 6 1.104843 3 110.559 2 27.591 0

CBS-QB3

H,0,-1.1277574562,0.7329815786,-1.2295563914
C,0,-1.1475224903,0.2159505302,-0.2767764766
C,0,-0.0324307356,-0.5219010167,0.1496883973
B,0,-0.092873805,1.0170660087,0.9860931287
H,0,-2.133634324,0.0153941618,0.1222274339
C,0,1.178873144,-0.7381545992,-0.7320217638
H,0,-0.2201218199,-1.2985473555,0.8823360205
H,0,-0.346317969,0.7983079387,2.1303924139
H,0,-1.0436314734,1.7010382867,0.5765639211
H,0,0.8674645096,1.622792913,0.6224596103
H,0,2.0898562472,-0.8252426646,-0.1363715676
H,0,1.0698908325,-1.6593978472,-1.3151020226
H,0,1.3151009683,0.0919734591,-1.4287560035

E(ZPE)= 0.110205
E(SCF)= -143.494323
DE(CBS)= -0.062661
DE(CCSD)= -0.019988
DE(Empirical)= -0.034498
CBS-QB3 (0 K)= -144.180250
CBS-QB3 Enthalpy= -144.174072
E(Thermal)= 0.115438
DE(MP2)= -0.649007
DE(MP34)= -0.053228
DE(Int)= 0.023250

CBS-QB3 Energy= -144.175016

CBS-QB3 Free Energy= -144.207275

G3B3

[For the structure, see the B3LYP/6-31G* structure.)

E(ZPE)= 0.108050	E(Thermal)= 0.113357
E(QCISD(T))= -144.007671	E(Empiric)= -0.081120
DE(Plus)= -0.007465	DE(2DF)= -0.158735
E(Delta-G3)= -0.217436	E(G3-Empiric)= -0.081120
G3(0 K)= -144.364378	G3 Energy= -144.359071
G3 Enthalpy= -144.358127	G3 Free Energy=-144.391452

2a-3‡ Complex

B3LYP/6-31G*

E(RB+HF-LYP) = -144.539357105

Zero-point correction= 0.112647
Thermal correction to Energy= 0.118647
Thermal correction to Enthalpy= 0.119591
Thermal correction to Gibbs Free Energy= 0.084705
Sum of electronic and ZPE= -144.426711
Sum of electronic and thermal Energies= -144.420710
Sum of electronic and thermal Enthalpies= -144.419766
Sum of electronic and thermal Free Energies= -144.454652

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.452	21.077	73.425

C,0,0.7189561102,0.1466768588,-0.0381739232
C,0,-0.0566114873,0.0260728684,1.2451971855
C,0,0.5251544697,-0.2100977073,2.4711681898
B,0,0.1615822449,1.6176149838,2.3533290533
H,0,0.2504607597,0.8512956472,-0.7307345184
H,0,0.7542275739,-0.8364253602,-0.5262663047
H,0,-1.1300998262,-0.1183810309,1.1496768995
H,0,1.6028157191,-0.30273307,2.5576554855
H,0,-0.0576625274,-0.600488837,3.2968445932
H,0,-0.4943900004,1.9992602463,1.4040662397
H,0,1.2673709792,2.0799462464,2.2979274579
H,0,-0.5158903408,1.732259903,3.337287817

H,0,1.7463623253,0.4713112517,0.1501338247

MP4/cc-pvdz

MP4SDTQ=-144.0828456

Zero-point correction= 0.111910
Thermal correction to Energy= 0.118023
Thermal correction to Enthalpy= 0.118967
Thermal correction to Gibbs Free Energy= 0.083710
Sum of electronic and ZPE= -143.970936
Sum of electronic and thermal Energies= -143.964823
Sum of electronic and thermal Enthalpies= -143.963879
Sum of electronic and thermal Free Energies= -143.999135

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.060	21.371	74.204

C
C,1,cc2
C,2,cc3,1,ccc3
B,3,bc4,2,bcc4,1,dih4,0
H,1,hc5,2,hcc5,3,dih5,0
H,1,hc6,2,hcc6,3,dih6,0
H,2,hc7,3,hcc7,4,dih7,0
H,3,hc8,2,hcc8,1,dih8,0
H,3,hc9,2,hcc9,1,dih9,0
H,4,hb10,3,hbc10,2,dih10,0
H,4,hb11,3,hbc11,2,dih11,0
H,4,hb12,3,hbc12,2,dih12,0
H,1,hc13,2,hcc13,3,dih13,0
Variables:
cc2=1.51184246
cc3=1.38839403
ccc3=123.13400036
bc4=1.90250934
bcc4=71.14918522
dih4=99.44225469
hc5=1.10314423
hcc5=111.50877532
dih5=-147.36430819
hc6=1.10710544

hcc6=108.77040144
dih6=93.02814868
hc7=1.09844942
hcc7=118.1090008
dih7=-95.03376053
hc8=1.0952153
hcc8=120.12168947
dih8=2.29374075
hc9=1.09333262
hcc9=120.72978846
dih9=-162.64099522
hb10=1.22769768
hbc10=116.91843991
dih10=7.03716189
hb11=1.21386036
hbc11=99.86567219
dih11=-112.59727318
hb12=1.21331724
hbc12=97.66733871
dih12=123.73186656
hc13=1.10430292
hcc13=110.55021844
dih13=-26.08591265

CCSD(T)/aug-cc-pvdz

CCSD(T)= -0.14411182005D+03

C
C 1 1.513503
C 2 1.380704 1 123.920
B 3 1.991632 2 71.912 1 94.866 0
H 1 1.103181 2 111.139 3 -136.796 0
H 1 1.106619 2 108.773 3 104.134 0
H 2 1.096963 3 118.309 4 -95.868 0
H 3 1.095278 2 120.642 1 1.944 0
H 3 1.092857 2 120.921 1 -166.917 0
H 4 1.220484 3 116.842 2 22.782 0
H 4 1.212188 3 100.272 2 -101.809 0
H 4 1.213877 3 91.114 2 137.842 0
H 1 1.103138 2 110.855 3 -15.478 0

CBS-QB3

C,0,0.3609322288,-0.2650980626,-1.5003355153
C,0,-0.4103744126,-0.3794297387,-0.2165377184
C,0,0.1739274394,-0.6198006066,1.0049370999
B,0,-0.1938770818,1.2029660315,0.8988954357
H,0,-0.1109819641,0.4293883913,-2.1967054482
H,0,0.3978340192,-1.2506221122,-1.9778665718
H,0,-1.4822831589,-0.518517468,-0.3080225814
H,0,1.2491873859,-0.7137924204,1.0854850563
H,0,-0.4073409828,-1.0069305518,1.8292577886
H,0,-0.8302342726,1.5815275521,-0.0612971185
H,0,0.9071749991,1.6676591732,0.8576016184
H,0,-0.8866271833,1.319663796,1.8665373648
H,0,1.3857450332,0.0627639296,-1.3178504845

E(ZPE)= 0.110293
E(SCF)= -143.504064
DE(CBS)= -0.062032
DE(CCSD)= -0.019722
DE(Empirical)= -0.034549
CBS-QB3 (0 K)= -144.183879
CBS-QB3 Enthalpy= -144.176850
E(Thermal)= 0.116377
DE(MP2)= -0.642059
DE(MP34)= -0.054892
DE(Int)= 0.023147

CBS-QB3 Energy= -144.177795
CBS-QB3 Free Energy= -144.211861

G3B3

[For the structure, see the B3LYP/6-31G* structure.)

E(ZPE)= 0.108139	E(Thermal)= 0.114312
E(QCISD(T))= -144.011434	E(Empiric)= -0.081120
DE(Plus)= -0.007458	DE(2DF)= -0.158253
E(Delta-G3)= -0.217978	E(G3-Empiric)= -0.081120
G3(0 K)= -144.368104	G3 Energy= -144.361932
G3 Enthalpy= -144.360988	G3 Free Energy= -144.396188

2a-4‡ Transition Structure

B3LYP/6-31G*

See technical comments.
E(RB+HF-LYP) = -376.985647856

Zero-point correction= 0.228778
Thermal correction to Energy= 0.242076
Thermal correction to Enthalpy= 0.243020
Thermal correction to Gibbs Free Energy= 0.184344
Sum of electronic and ZPE= -376.756870
Sum of electronic and thermal Energies= -376.743572
Sum of electronic and thermal Enthalpies= -376.742627
Sum of electronic and thermal Free Energies= -376.801304

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.905	43.724	123.495

C,0,-4.242429518,0.0919422872,-0.7950108234
C,0,-3.6331129172,-0.5165493056,0.4337706747
C,0,-3.2550276056,0.1605374753,1.5297891303
B,0,-1.0782490767,0.091252537,0.1159527129
H,0,-5.2593806016,-0.2933807132,-0.9483133399
H,0,-3.6617472836,-0.1654937334,-1.6884887876
H,0,-3.5344289273,-1.6017220941,0.4319292214
H,0,-3.3561366761,1.2412751119,1.5933208091
H,0,-2.8693383951,-0.346697153,2.4085006321
H,0,-0.5556114871,0.1147031658,1.1926825779
H,0,-1.3577354828,1.1099102688,-0.4403052073
H,0,-1.1642763237,-0.9513027325,-0.4631462692
H,0,-4.2937340958,1.1826157506,-0.7212127078
O,0,1.5011987129,0.2738226838,-1.0247032572
C,0,2.1839271621,-0.9852936056,-0.8956922655
C,0,2.2270695052,1.2789969554,-0.3137118495
C,0,2.9430963149,0.5337215039,0.8127199089
H,0,2.9521889958,1.7715884674,-0.982933169
H,0,1.507548457,2.0269735877,0.0303234195
C,0,3.3418334164,-0.7716400995,0.1029433794
H,0,1.4565067866,-1.7223673433,-0.5382008699
H,0,2.5430925065,-1.3080704327,-1.8818149042
H,0,2.2412876128,0.3314020908,1.6295418203
H,0,3.7981010851,1.0839453438,1.2185121917
H,0,3.4624557006,-1.615614813,0.7888779913

H,0,4.2906901347,-0.6380052034,-0.4295720192

2a-5‡ Variational Transition State

B3LYP/6-31G*

E(RB+HF-LYP) = -144.523976652

Zero-point correction= 0.107771
Thermal correction to Energy= 0.114636
Thermal correction to Enthalpy= 0.115580
Thermal correction to Gibbs Free Energy= 0.076800
Sum of electronic and ZPE= -144.416206
Sum of electronic and thermal Energies= -144.409340
Sum of electronic and thermal Enthalpies= -144.408396
Sum of electronic and thermal Free Energies= -144.447176

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	71.935	21.135	81.619

1	6	1.804733	-0.709183	0.170106
2	6	0.839020	0.252441	-0.460550
3	6	0.082688	1.133617	0.201331
4	5	-2.851904	-0.550134	0.016632
5	1	2.827028	-0.530462	-0.189709
6	1	1.557781	-1.746893	-0.090215
7	1	0.776538	0.220380	-1.549202
8	1	0.116733	1.213306	1.286395
9	1	-0.578890	1.822263	-0.316660
10	1	-3.258990	0.481010	-0.427460
11	1	-2.796535	-0.710540	1.198415
12	1	-2.549386	-1.438474	-0.721537
13	1	1.806593	-0.621171	1.261489

2a-5‡ Complex

B3LYP/6-31G*

E(RB+HF-LYP) = -259.096303497

Zero-point correction= 0.150614

Thermal correction to Energy= 0.157553
Thermal correction to Enthalpy= 0.158497
Thermal correction to Gibbs Free Energy= 0.119856
Sum of electronic and ZPE= -258.945690
Sum of electronic and thermal Energies= -258.938751
Sum of electronic and thermal Enthalpies= -258.937807
Sum of electronic and thermal Free Energies= -258.976448

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	98.866	25.093	81.327

C,0,-1.6904691648,1.0035767143,-0.2769372581
O,0,-0.2785927146,0.6604841196,-0.3339671837
C,0,0.5371677343,1.8342560356,-0.0163629084
C,0,-0.4505713973,3.0052286477,0.0788749555
C,0,-1.7088625227,2.4816167557,-0.639370736
H,0,-2.199796678,0.3404577503,-0.9768840103
H,0,-2.0526565799,0.811756002,0.7398350783
H,0,1.0662161019,1.6283698732,0.9159457328
H,0,1.2576893737,1.9321963974,-0.8315754163
H,0,-0.6792237432,3.2238722372,1.127244078
H,0,-0.0508824675,3.9168417604,-0.3738267582
H,0,-2.6254063435,2.9784059947,-0.3088943267
H,0,-1.6213166511,2.6077849379,-1.7241214316
H,0,-0.0121608047,-0.5779876672,1.5498207304
B,0,0.1695736986,-0.7637682176,0.3632502645
H,0,1.3281474394,-0.8731835523,0.0419047318
H,0,-0.5790068106,-1.5640063888,-0.1439965021

Table A1. Summary of Single-Point Energies on the CCSD(T)/aug-cc-pvdz geometries.

Structure\Method Basis Set	CCSD(T)/aug-cc-pvdz
BH3	-26.512760
propene	-117.578765
complex (**3**)	-144.111820
TS **1**	-144.110806
TS **2**	-144.106709

	CCSD(T)/cc-pvtz
BH3	-26.537419
propene	-117.681375
complex (**3**)	-144.239881
TS **1**	-144.239816
TS **2**	-144.235997
	CCSD(T)/aug-cc-pvtz
BH3	-26.538792
propene	-117.689360
complex (**3**)	-144.249993
TS **1**	-144.249845
TS **2**	-144.245956
	CCSD(T)/cc-pvqz
BH3	-26.544712
propene	-117.715774
complex (**3**)	-144.281877
TS **1**	-144.282026
TS **2**	-144.278228
	CCSD(T)/aug-cc-pvqz
BH3	-26.545123
propene	-117.718677
complex (**3**)	-144.285478
TS **1**	-144.285580
TS **2**	-144.281762
	BD(TQ)-aug-cc-pvdz
BH3	-26.513094
propene	-117.579602
complex (**3**)	-144.112664
TS **1**	-144.111485
TS **2**	-144.107399

A. 2. Theoretical Structures from " Isotope Effects, Dynamics, and the Nature of Selectivity In The Hydroboration of Styrene"

3a-1 Starting Material
B3LYP/6-31+G**
E(RB+HF-LYP) = -309.673926771

Zero-point correction= 0.133273 (Hartree/Particle)
Thermal correction to Energy= 0.140040
Thermal correction to Enthalpy= 0.140984
Thermal correction to Gibbs Free Energy= 0.101970
Sum of electronic and ZPE= -309.540654
Sum of electronic and thermal Energies= -309.533887
Sum of electronic and thermal Enthalpies= -309.532943
Sum of electronic and thermal Free Energies= -309.571956

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	87.876	26.128	82.111

C,0,0.0921466462,-0.2706446737,-0.2767502824
C,0,1.5028338241,-0.629293789,-0.5070690635
C,0,2.5340032478,0.1992891396,-0.7300210775
H,0,1.7046573068,-1.7000051939,-0.4890690547
H,0,2.4263287109,1.2795372313,-0.7652237435
H,0,3.5343819503,-0.1908478592,-0.8865168824
C,0,-0.8432476497,-1.2989120109,-0.0620697378
C,0,-2.1923022847,-1.0163242552,0.1610563162
C,0,-2.6363008942,0.3074077996,0.1742481189
C,0,-1.7182600488,1.3431528871,-0.0376840997
C,0,-0.3727914334,1.0586444334,-0.2600960889
H,0,-0.5048423054,-2.3322010049,-0.0709307815
H,0,-2.8940677846,-1.8293387025,0.3241281564
H,0,-3.6845556143,0.5325765904,0.347369073
H,0,-2.0543405396,2.3762405257,-0.0291608579
H,0,0.3219078686,1.8769988822,-0.4220719947

B3LYP/6-31G*
E(RB+HF-LYP) = -309.648258911

Zero-point correction= 0.133731 (Hartree/Particle)
Thermal correction to Energy= 0.140501
Thermal correction to Enthalpy= 0.141445

Thermal correction to Gibbs Free Energy= 0.102253
Sum of electronic and ZPE= -309.514528
Sum of electronic and thermal Energies= -309.507758
Sum of electronic and thermal Enthalpies= -309.506814
Sum of electronic and thermal Free Energies= -309.546006

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	88.166	26.029	82.487

C,0,0.0917131662,-0.2706957746,-0.2767082671
C,0,1.5011241331,-0.6287849265,-0.5068137668
C,0,2.5301323713,0.1985699369,-0.7291500215
H,0,1.7017773869,-1.7002571053,-0.4886993411
H,0,2.4230813524,1.2794101897,-0.7643127119
H,0,3.5323059474,-0.1883841033,-0.8861504761
C,0,-0.8431468721,-1.2977621807,-0.0620148622
C,0,-2.1903399994,-1.0152896778,0.1608039443
C,0,-2.6335423026,0.3071695931,0.1737500546
C,0,-1.7167332117,1.3417474711,-0.0380936827
C,0,-0.3728883424,1.0574661203,-0.2602402257
H,0,-0.5038133994,-2.3312988054,-0.070899002
H,0,-2.8925460343,-1.8286416352,0.3241070539
H,0,-3.6823294063,0.5325797892,0.3469578462
H,0,-2.0528069782,2.3754316452,-0.0297493773
H,0,0.323563189,1.8750194632,-0.4226491647

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.128381	E(Thermal)=	0.135387
E(QCISD(T))=	-308.693658	E(Empiric)=	-0.135200
DE(Plus)=	-0.018855	DE(2DF)=	-0.243769
E(Delta-G3)=	-0.433513	E(G3-Empiric)=	-0.135200
G3(0 K)=	-309.396614	G3 Energy=	-309.389609
G3 Enthalpy=	-309.388665	G3 Free Energy=	-309.428258

For Anharmonic Corrections of 3a-1
Zero-point vibrational energy 351109.7 (Joules/Mol)
83.91722 (Kcal/Mol)

Vibrational temperatures:	62.17	299.32	341.20	595.14	645.98
(Kelvin)	646.44	807.34	913.12	942.93	1027.13
	1136.47	1151.57	1229.59	1326.70	1332.70
	1387.36	1428.13	1462.19	1493.06	1506.88
	1533.87	1613.77	1716.85	1752.59	1780.71

1918.87 1964.40 1980.40 2118.31 2159.59
2226.51 2353.99 2392.63 2465.76 4531.02
4563.71 4570.91 4580.95 4595.18 4607.86
4620.05 4674.14

Zero-point correction= 0.133731 (Hartree/Particle)
Thermal correction to Energy= 0.140501
Thermal correction to Enthalpy= 0.141445
Thermal correction to Gibbs Free Energy= 0.102253
Sum of electronic and zero-point Energies= -309.514528
Sum of electronic and thermal Energies= -309.507758
Sum of electronic and thermal Enthalpies= -309.506814
Sum of electronic and thermal Free Energies= -309.546006

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.166	26.029	82.487

ZPE(harm) = 0.35111D+03 kJ/mol ZPE(anh)= 0.34663D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.78568D-60	0.35136D-59	
QZvib	0.25523D+02	0.18724D+02	
Energy	0.36888D+03	0.36448D+03	kJ/mol
Enthalpy	0.37136D+03	0.36696D+03	kJ/mol
Entropy	0.34513D+03	0.34281D+03	J/(mol K)
Sp.Heat(V)	0.10890D+03	0.11058D+03	J/(mol K)
Sp.Heat(P)	0.11722D+03	0.11889D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.78568D-60	0.35136D-59	
QZvib	0.25523D+02	0.18724D+02	
Energy	0.36888D+03	0.36448D+03	kJ/mol
Enthalpy	0.37136D+03	0.36696D+03	kJ/mol
Entropy	0.34513D+03	0.34281D+03	J/(mol K)
Sp.Heat(V)	0.10890D+03	0.11058D+03	J/(mol K)
Sp.Heat(P)	0.11722D+03	0.11889D+03	J/(mol K)

3a-2 Complex
B3LYP/6-31+G**
E(RB+HF-LYP) = -336.303440564
Zero-point correction= 0.164927 (Hartree/Particle)
Thermal correction to Energy= 0.173932
Thermal correction to Enthalpy= 0.174876
Thermal correction to Gibbs Free Energy= 0.130945
Sum of electronic and ZPE= -336.138513
Sum of electronic and thermal Energies= -336.129509
Sum of electronic and thermal Enthalpies= -336.128565
Sum of electronic and thermal Free Energies= -336.172495

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.144	34.710	92.459

C,0,0.0618015094,-0.2570668086,-0.1839641346
C,0,1.4867561317,-0.6066045973,-0.3566361517
C,0,2.4947275093,0.2376228408,-0.770857676
B,0,2.6595451206,0.1513283686,1.1095174906
H,0,1.7027196377,-1.6708006625,-0.319870494
H,0,2.2884146933,1.2670801228,-1.037504808
H,0,3.4179179481,-0.1750673789,-1.1558613359
H,0,3.792186059,-0.2426711054,1.1635763291
H,0,1.940478454,-0.6193328289,1.7044863678
H,0,2.3690765685,1.2822841861,1.3867083984
C,0,-0.8689720875,-1.2975575367,-0.0291406092
C,0,-2.2316980914,-1.0257560505,0.0972495189
C,0,-2.6835565103,0.2959918411,0.0824373098
C,0,-1.764379916,1.3409738842,-0.0611290224
C,0,-0.403991326,1.0687991324,-0.1947574006
H,0,-0.5197472943,-2.3267701483,-0.0079504426
H,0,-2.9371517598,-1.8434298849,0.2113978577
H,0,-3.7429561703,0.5120709807,0.1842284517
H,0,-2.1088809675,2.3708836195,-0.0668396772
H,0,0.2960004913,1.8915820259,-0.2946399718

B3LYP/6-31G*
E(RB+HF-LYP) = -336.276253257

Zero-point correction= 0.165773 (Hartree/Particle)
Thermal correction to Energy= 0.174720
Thermal correction to Enthalpy= 0.175664
Thermal correction to Gibbs Free Energy= 0.131881

Sum of electronic and ZPE= -336.110480
Sum of electronic and thermal Energies= -336.101533
Sum of electronic and thermal Enthalpies= -336.100589
Sum of electronic and thermal Free Energies= -336.144373

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.639	34.493	92.151

C,0,0.0754942791,-0.2555840402,-0.1904538863
C,0,1.494937163,-0.6122793536,-0.3779750911
C,0,2.5098123897,0.2272811177,-0.7788702803
B,0,2.6608981568,0.1377985514,1.1112107321
H,0,1.7034968509,-1.6787640664,-0.3553214894
H,0,2.3170560893,1.2634969327,-1.0313218894
H,0,3.4308071766,-0.1886248351,-1.1673714389
H,0,3.8147417575,-0.1971660919,1.1437907109
H,0,1.9925560373,-0.684290829,1.6977773311
H,0,2.3226766561,1.2525787802,1.400410071
C,0,-0.8592424543,-1.2907957779,-0.033346423
C,0,-2.2175833905,-1.0119875909,0.1054768712
C,0,-2.6609854338,0.3111769084,0.1010127771
C,0,-1.7384565034,1.3510002859,-0.045061472
C,0,-0.3826488768,1.0721369363,-0.1928988425
H,0,-0.5148984845,-2.3222812974,-0.0217221569
H,0,-2.9272064224,-1.8264423856,0.2213934503
H,0,-3.7187459982,0.5328660275,0.2129432528
H,0,-2.0774908461,2.3832304689,-0.0436667168
H,0,0.3230718537,1.8902102591,-0.2955555099

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.159142	E(Thermal)=	0.168401
E(QCISD(T))=	-335.193984	E(Empiric)=	-0.155480
DE(Plus)=	-0.019763	DE(2DF)=	-0.285792
E(Delta-G3)=	-0.481857	E(G3-Empiric)=	-0.155480
G3(0 K)=	-335.977734 G3	Energy=	-335.968475
G3 Enthalpy=	-335.967531	G3 Free Energy=	-336.011882

For Anharmonic Corrections of 3a-2

Vibrational temperatures:	76.39 129.89 214.32 311.22 345.32
(Kelvin)	424.44 561.17 596.62 686.61 764.67
	829.99 912.39 1009.63 1056.09 1101.78
	1131.85 1192.20 1216.17 1232.72 1340.82
	1391.93 1435.69 1437.62 1464.80 1483.56

1524.67 1563.15 1592.47 1616.32 1673.81
1698.18 1720.26 1753.05 1770.13 1902.51
1955.49 1977.14 2113.17 2164.52 2225.83
2324.73 2369.93 2393.28 3605.73 3673.37
3791.09 4578.24 4589.94 4594.21 4598.54
4605.53 4620.25 4631.17 4719.33

Zero-point correction= 0.165773 (Hartree/Particle)
Thermal correction to Energy= 0.174720
Thermal correction to Enthalpy= 0.175664
Thermal correction to Gibbs Free Energy= 0.131882
Sum of electronic and zero-point Energies= -336.110480
Sum of electronic and thermal Energies= -336.101533
Sum of electronic and thermal Enthalpies= -336.100589
Sum of electronic and thermal Free Energies= -336.144372

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.638	34.493	92.148

ZPE(harm) = 0.43524D+03 kJ/mol ZPE(anh)= 0.42915D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.96785D-74	0.23671D-72	
QZvib	0.17219D+03	0.36078D+03	
Energy	0.45873D+03	0.45338D+03	kJ/mol
Enthalpy	0.46121D+03	0.45586D+03	kJ/mol
Entropy	0.38555D+03	0.39421D+03	J/(mol K)
Sp.Heat(V)	0.14432D+03	0.14761D+03	J/(mol K)
Sp.Heat(P)	0.15263D+03	0.15593D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.96785D-74	0.23671D-72	
QZvib	0.17219D+03	0.36078D+03	
Energy	0.45873D+03	0.45338D+03	kJ/mol
Enthalpy	0.46121D+03	0.45586D+03	kJ/mol
Entropy	0.38555D+03	0.39421D+03	J/(mol K)
Sp.Heat(V)	0.14432D+03	0.14761D+03	J/(mol K)
Sp.Heat(P)	0.15263D+03	0.15593D+03	J/(mol K)

3a-3‡ Transition Structure
B3LYP/6-31+G**
E(RB+HF-LYP) = -336.302671883

Zero-point correction= 0.164816 (Hartree/Particle)
Thermal correction to Energy= 0.172849
Thermal correction to Enthalpy= 0.173793
Thermal correction to Gibbs Free Energy= 0.132095
Sum of electronic and ZPE= -336.137856
Sum of electronic and thermal Energies= -336.129823
Sum of electronic and thermal Enthalpies= -336.128878
Sum of electronic and thermal Free Energies= -336.170577

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.465	32.204	87.762

C,0,0.1156962469,-0.262411453,-0.105698154
C,0,1.5526195817,-0.6141868776,-0.2367761553
C,0,2.549489631,0.2319644852,-0.7628829929
B,0,2.7727210633,0.2098746192,0.9612985473
H,0,1.7555582974,-1.6816208911,-0.2288454871
H,0,2.2704099423,1.2138997838,-1.1273286462
H,0,3.4036367233,-0.218026949,-1.2544296814
H,0,3.8290322438,-0.319024007,1.1649049207
H,0,1.9557936378,-0.5431501692,1.5012338622
H,0,2.4751931625,1.2995671036,1.3630011642
C,0,-0.826953723,-1.2988019065,-0.0207691192
C,0,-2.1917585113,-1.0177381101,0.0645802563
C,0,-2.6316844133,0.3078132846,0.0803860233
C,0,-1.6989308446,1.3477629697,0.0073017715
C,0,-0.3364069489,1.0669362952,-0.0873998091
H,0,-0.4884139869,-2.3319515464,-0.0249638631
H,0,-2.9077283884,-1.8322297732,0.1227704306
H,0,-3.692271696,0.5303844513,0.1510800285
H,0,-2.0339474361,2.3806966617,0.0256059293
H,0,0.3762354184,1.8838020286,-0.1326190257

B3LYP/6-31G*
E(RB+HF-LYP) = -336.274896670

Zero-point correction= 0.165690 (Hartree/Particle)
Thermal correction to Energy= 0.173631

Thermal correction to Enthalpy= 0.174575
Thermal correction to Gibbs Free Energy= 0.133066
Sum of electronic and ZPE= -336.109207
Sum of electronic and thermal Energies= -336.101266
Sum of electronic and thermal Enthalpies= -336.100322
Sum of electronic and thermal Free Energies= -336.141830

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.955	31.856	87.362

C,0,0.115870498,-0.2641827237,-0.0951787174
C,0,1.5532142162,-0.6157677568,-0.22025579
C,0,2.5507976231,0.2327558473,-0.7558410219
B,0,2.7800836653,0.2244964092,0.9480616088
H,0,1.754535667,-1.6841977519,-0.2202283399
H,0,2.2585569659,1.2048278221,-1.138273744
H,0,3.3917116269,-0.2239244109,-1.2655711972
H,0,3.8298017173,-0.311403259,1.1700591345
H,0,1.9585220402,-0.5449420231,1.4763939046
H,0,2.4649796257,1.3018536717,1.3704342064
C,0,-0.8273890964,-1.2988796977,-0.0178142614
C,0,-2.1906749898,-1.0163368001,0.0598545292
C,0,-2.6281904469,0.308467154,0.0761868762
C,0,-1.6951385865,1.3467034002,0.010960251
C,0,-0.334058599,1.0648308879,-0.0784310921
H,0,-0.4891722089,-2.3326233017,-0.0236316451
H,0,-2.9083922468,-1.8303781251,0.1118427504
H,0,-3.6894265693,0.5322433477,0.1413007116
H,0,-2.0293114202,2.3804217172,0.0289773151
H,0,0.3819705181,1.8795955926,-0.1183954787

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.159062	E(Thermal)=	0.167305
E(QCISD(T))=	-335.193073	E(Empiric)=	-0.155480
DE(Plus)=	-0.020134	DE(2DF)=	-0.286159
E(Delta-G3)=	-0.481392	E(G3-Empiric)=	-0.155480
G3(0 K)=	-335.977176	G3 Energy=	-335.968933
G3 Enthalpy=	-335.967989	G3 Free Energy=	-336.010014

For Anharmonic Corrections of 3a-3‡
Vibrational temperatures: 77.17 205.52 276.96 383.93 481.56
(Kelvin) 567.17 598.40 766.57 817.10 886.80
918.05 1006.69 1020.11 1107.27 1121.27

1177.54 1223.79 1317.28 1376.69 1389.43
1426.74 1462.39 1473.17 1508.60 1525.33
1575.89 1607.29 1641.34 1675.01 1716.64
1720.34 1754.25 1766.68 1870.97 1940.96
1974.29 2086.32 2156.02 2221.32 2246.07
2364.78 2395.78 3369.77 3728.34 3880.30
4566.50 4570.27 4578.04 4590.68 4595.14
4603.21 4619.84 4690.85

Zero-point correction= 0.165660 (Hartree/Particle)
Thermal correction to Energy= 0.173712
Thermal correction to Enthalpy= 0.174656
Thermal correction to Gibbs Free Energy= 0.132845
Sum of electronic and zero-point Energies= -336.106590
Sum of electronic and thermal Energies= -336.098538
Sum of electronic and thermal Enthalpies= -336.097594
Sum of electronic and thermal Free Energies= -336.139405

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.006	32.063	87.998

ZPE(harm) = 0.43494D+03 kJ/mol ZPE(anh)= 0.42974D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.35669D-74	0.17365D-73	
QZvib	0.56285D+02	0.33693D+02	
Energy	0.45608D+03	0.45085D+03	kJ/mol
Enthalpy	0.45856D+03	0.45333D+03	kJ/mol
Entropy	0.37650D+03	0.37213D+03	J/(mol K)
Sp.Heat(V)	0.13415D+03	0.13605D+03	J/(mol K)
Sp.Heat(P)	0.14247D+03	0.14436D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.35669D-74	0.17365D-73	
QZvib	0.56285D+02	0.33693D+02	
Energy	0.45608D+03	0.45085D+03	kJ/mol
Enthalpy	0.45856D+03	0.45333D+03	kJ/mol
Entropy	0.37650D+03	0.37213D+03	J/(mol K)
Sp.Heat(V)	0.13415D+03	0.13605D+03	J/(mol K)
Sp.Heat(P)	0.14247D+03	0.14436D+03	J/(mol K)

3a-4‡ Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -336.272249885

H,0,-0.0631734007,-0.329557854,0.2771520423
C,0,0.0209157045,-0.0868781511,1.3318767572
C,0,1.2740618152,0.2304165168,1.8946148893
B,0,0.3109324303,1.68597962,1.6903807553
H,0,-0.7816772052,-0.455938313,1.9605904742
C,0,2.5598728429,0.1447804386,1.1428141652
H,0,1.3740932325,0.0666813757,2.9629223854
H,0,-0.0145725245,2.0653536382,2.7757073967
H,0,-0.7545635987,1.4381086647,1.0950092168
H,0,0.904619179,2.3576533186,0.9030199749
C,0,3.7350516727,-0.1438490697,1.8529341439
C,0,4.9620881997,-0.2679153043,1.1960804006
C,0,5.0361619008,-0.1047910664,-0.1883419594
C,0,3.8722956391,0.1900248464,-0.9064347338
C,0,2.6495669498,0.3184848102,-0.2480087572
H,0,3.6876331438,-0.273869652,2.9313282921
H,0,5.857750209,-0.4914838669,1.7687365958
H,0,5.9878769456,-0.2001760968,-0.7025557878
H,0,3.9183445416,0.329270985,-1.982894753
H,0,1.7644523225,0.57633516,-0.8226514987

B3LYP/6-31G*
E(RB+HF-LYP) = -336.272249899

Zero-point correction= 0.165659 (Hartree/Particle)
Thermal correction to Energy= 0.173711
Thermal correction to Enthalpy= 0.174655
Thermal correction to Gibbs Free Energy= 0.132844
Sum of electronic and ZPE= -336.106591
Sum of electronic and thermal Energies= -336.098539
Sum of electronic and thermal Enthalpies= -336.097595
Sum of electronic and thermal Free Energies= -336.139406

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.005	32.063	88.000

H,0,-0.0666766481,-0.3186188287,0.2746762435
C,0,0.0216991963,-0.0809077961,1.330671942
C,0,1.2763777345,0.215317805,1.8921403455
B,0,0.304085464,1.6951561133,1.684318349
H,0,-0.7835619958,-0.4493737543,1.9573093623
C,0,2.5610688287,0.1400624393,1.1420773346
H,0,1.3744809578,0.0594845822,2.9620560537
H,0,-0.0005549228,2.0670005675,2.7786668307
H,0,-0.7623979144,1.4390004004,1.1016403529
H,0,0.9098552846,2.358977241,0.8989498414
C,0,3.7355387231,-0.1442428325,1.8526431428
C,0,4.9614516116,-0.2652030721,1.1969928396
C,0,5.0350432103,-0.1026073239,-0.1859218525
C,0,3.8721690838,0.188099142,-0.9044495767
C,0,2.6499819026,0.3115633966,-0.2480097319
H,0,3.6868417886,-0.2744594367,2.931458342
H,0,5.8579617904,-0.4862206008,1.7702939046
H,0,5.9878200821,-0.1952114568,-0.6998707207
H,0,3.9182443817,0.3261471733,-1.9815699643
H,0,1.7623014409,0.5646662413,-0.8217930386

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.159032	E(Thermal)=	0.167386
E(QCISD(T))=	-335.190970	E(Empiric)=	-0.155480
DE(Plus)=	-0.019893	DE(2DF)=	-0.286390
E(Delta-G3)=	-0.481456	E(G3-Empiric)=	-0.155480
G3(0 K)=	-335.975157	G3 Energy=	-335.966803
G3 Enthalpy=	-335.965859	G3 Free Energy=	-336.008191

For Anharmonic Corrections of 3a-4[‡]

Vibrational temperatures: 90.12 196.45 280.43 411.50 555.98
(Kelvin) 567.27 599.17 763.14 807.85 908.19
941.95 1018.40 1064.98 1109.91 1136.37
1168.57 1232.57 1291.53 1341.40 1395.10
1438.28 1463.34 1469.60 1489.90 1526.32
1553.00 1606.24 1637.51 1687.91 1714.62
1719.87 1753.75 1767.08 1848.40 1943.35
1974.26 2076.20 2161.65 2220.58 2246.13
2365.91 2394.56 3357.25 3669.43 3821.72
4568.48 4574.25 4583.89 4589.50 4604.06
4619.37 4630.43 4683.37

Zero-point correction=	0.165690 (Hartree/Particle)
Thermal correction to Energy=	0.173630

Thermal correction to Enthalpy= 0.174574
Thermal correction to Gibbs Free Energy= 0.133066
Sum of electronic and zero-point Energies= -336.109207
Sum of electronic and thermal Energies= -336.101267
Sum of electronic and thermal Enthalpies= -336.100322
Sum of electronic and thermal Free Energies= -336.141831

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	108.955	31.856	87.362

ZPE(harm) = 0.43502D+03 kJ/mol ZPE(anh)= 0.42900D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.28130D-74	0.37371D-73	
QZvib	0.45804D+02	0.53774D+02	
Energy	0.45587D+03	0.45036D+03	kJ/mol
Enthalpy	0.45834D+03	0.45284D+03	kJ/mol
Entropy	0.37384D+03	0.37689D+03	J/(mol K)
Sp.Heat(V)	0.13329D+03	0.13666D+03	J/(mol K)
Sp.Heat(P)	0.14160D+03	0.14498D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.28130D-74	0.37371D-73	
QZvib	0.45804D+02	0.53774D+02	
Energy	0.45587D+03	0.45036D+03	kJ/mol
Enthalpy	0.45834D+03	0.45284D+03	kJ/mol
Entropy	0.37384D+03	0.37689D+03	J/(mol K)
Sp.Heat(V)	0.13329D+03	0.13666D+03	J/(mol K)
Sp.Heat(P)	0.14160D+03	0.14498D+03	J/(mol K)

3a-5‡ Variational Transition State
B3LYP/6-31+G**

E(RB+HF-LYP) = -336.293532966

Zero-point correction= 0.160956 (Hartree/Particle)
Thermal correction to Energy= 0.171340
Thermal correction to Enthalpy= 0.172284
Thermal correction to Gibbs Free Energy= 0.122936
Sum of electronic and zero-point Energies= -336.132577
Sum of electronic and thermal Energies= -336.122193

Sum of electronic and thermal Enthalpies= -336.121249
Sum of electronic and thermal Free Energies= -336.170597

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	107.518	36.238	103.862

C,0,0.11625,-0.45682,-0.19777
C,0,-1.15493,-1.14126,-0.48473
C,0,-2.09714,-1.52743,0.39038
B,0,-3.88458,1.28077,-0.09033
H,0,-1.32679,-1.3481,-1.54111
H,0,-2.00814,-1.36912,1.46203
H,0,-2.99051,-2.04317,0.05366
H,0,-3.05002,2.00461,-0.542
H,0,-4.03557,1.20837,1.09225
H,0,-4.60568,0.67041,-0.82116
C,0,0.94071,-0.08154,-1.27226
C,0,2.14402,0.58983,-1.05959
C,0,2.55112,0.89741,0.23861
C,0,1.74748,0.52214,1.31994
C,0,0.54702,-0.14769,1.10569
H,0,0.62596,-0.3148,-2.28697
H,0,2.76137,0.87341,-1.90781
H,0,3.48689,1.42255,0.40971
H,0,2.05949,0.75416,2.33487
H,0,-0.06341,-0.4309,1.95829

B3LYP/6-31G*
E(RB+HF-LYP) = -336.264787260

Zero-point correction= 0.161409 (Hartree/Particle)
Thermal correction to Energy= 0.170974
Thermal correction to Enthalpy= 0.171918
Thermal correction to Gibbs Free Energy= 0.124884
Sum of electronic and ZPE= -336.103378
Sum of electronic and thermal Energies= -336.093813
Sum of electronic and thermal Enthalpies= -336.092869
Sum of electronic and thermal Free Energies= -336.139903

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	107.288	34.224	98.991

C,0,0.11625,-0.45682,-0.19777
C,0,-1.15493,-1.14126,-0.48473
C,0,-2.09714,-1.52743,0.39038
B,0,-3.88458,1.28077,-0.09033
H,0,-1.32679,-1.3481,-1.54111
H,0,-2.00814,-1.36912,1.46203
H,0,-2.99051,-2.04317,0.05366
H,0,-3.05002,2.00461,-0.542
H,0,-4.03557,1.20837,1.09225
H,0,-4.60568,0.67041,-0.82116
C,0,0.94071,-0.08154,-1.27226
C,0,2.14402,0.58983,-1.05959
C,0,2.55112,0.89741,0.23861
C,0,1.74748,0.52214,1.31994
C,0,0.54702,-0.14769,1.10569
H,0,0.62596,-0.3148,-2.28697
H,0,2.76137,0.87341,-1.90781
H,0,3.48689,1.42255,0.40971
H,0,2.05949,0.75416,2.33487
H,0,-0.06341,-0.4309,1.95829

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.154953	E(Thermal)=	0.164798
E(QCISD(T))=	-335.182528	E(Empiric)=	-0.155480
DE(Plus)=	-0.020410	DE(2DF)=	-0.282342
E(Delta-G3)=	-0.482004	E(G3-Empiric)=	-0.155480
G3(0 K)=	-335.967812	G3 Energy=	-335.957967
G3 Enthalpy=	-335.957023	G3 Free Energy=	-336.004617

3a-6 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -336.334353385

Zero-point correction= 0.166212 (Hartree/Particle)
Thermal correction to Energy= 0.175333
Thermal correction to Enthalpy= 0.176277
Thermal correction to Gibbs Free Energy= 0.131002
Sum of electronic and ZPE= -336.168141
Sum of electronic and thermal Energies= -336.159021
Sum of electronic and thermal Enthalpies= -336.158077
Sum of electronic and thermal Free Energies= -336.203352

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 110.023 34.006 95.290

H,0,1.3100522681,0.043228725,1.8114139371
C,0,0.4513150218,0.2222519593,1.1346465628
C,0,-0.3136955459,1.4849588006,1.554365241
H,0,-1.1337186454,1.6542759725,0.8433745993
B,0,1.094474442,0.2125987497,-0.2868342199
H,0,-0.1626315799,-0.6826372218,1.2658882356
H,0,1.1546564962,1.1990797842,-0.9646936282
H,0,1.5790131357,-0.7970167176,-0.7095805605
C,0,-0.8949537554,1.5137307752,2.9608006043
H,0,0.3495171015,2.3530736903,1.4358507177
C,0,-1.7066012045,2.5981588776,3.3382215275
C,0,-2.2548078091,2.6837970901,4.6175859926
C,0,-2.0030004699,1.6782830657,5.5577148309
C,0,-1.2011669057,0.5950247828,5.1987812512
C,0,-0.6543858274,0.5137732687,3.9121674801
H,0,-1.9100267385,3.3854440745,2.6150886786
H,0,-2.8791214992,3.5330246465,4.8816449372
H,0,-2.4285526357,1.7405128465,6.5551039117
H,0,-0.9982428535,-0.1941562323,5.9176910592
H,0,-0.0363449951,-0.3413779376,3.6593358417

B3LYP/6-31G*
E(RB+HF-LYP) = -336.307868190

Zero-point correction= 0.166999 (Hartree/Particle)
Thermal correction to Energy= 0.176125
Thermal correction to Enthalpy= 0.177069
Thermal correction to Gibbs Free Energy= 0.131926
Sum of electronic and ZPE= -336.140870
Sum of electronic and thermal Energies= -336.131743
Sum of electronic and thermal Enthalpies= -336.130799
Sum of electronic and thermal Free Energies= -336.175942

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 110.520 33.845 95.011
Zero-point correction= 0.166999 (Hartree/Particle)
Thermal correction to Energy= 0.176125
Thermal correction to Enthalpy= 0.177069
Thermal correction to Gibbs Free Energy= 0.131926

Sum of electronic and ZPE= -336.140870
Sum of electronic and thermal Energies= -336.131743
Sum of electronic and thermal Enthalpies= -336.130799
Sum of electronic and thermal Free Energies= -336.175942

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.520	33.845	95.011

H,0,0.1570693949,-0.6185372204,1.531718089
C,0,0.0113137832,0.313072499,0.9629255104
C,0,0.2877992469,1.5440536501,1.8556341387
H,0,0.1073933887,2.4548248872,1.2708808114
B,0,0.7375767526,0.2302172996,-0.4167460833
H,0,-1.0665212045,0.2772920243,0.7073913173
H,0,1.3295469743,1.1642258855,-0.8812815501
H,0,0.6752361877,-0.7779120625,-1.0617113088
C,0,-0.548719548,1.5737185198,3.11801257
H,0,1.3523222772,1.5577642819,2.1220591853
C,0,-1.8088724501,2.1873452718,3.1311429106
C,0,-2.600322258,2.1812726009,4.280452427
C,0,-2.1423913251,1.5587841631,5.4431437741
C,0,-0.8880515684,0.9460781135,5.4460745139
C,0,-0.1010805109,0.9557109997,4.2935856177
H,0,-2.1714163219,2.6801974312,2.2309398168
H,0,-3.5726365068,2.6674391261,4.2692736786
H,0,-2.7555323501,1.5555529449,6.3404278178
H,0,-0.5190077827,0.4642515699,6.3480252238
H,0,0.878071821,0.4806770145,4.3066185398

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.160319	E(Thermal)=	0.169736
E(QCISD(T))=	-335.227187	E(Empiric)=	-0.155480
DE(Plus)=	-0.019745	DE(2DF)=	-0.283922
E(Delta-G3)=	-0.481831	E(G3-Empiric)=	-0.155480
G3(0 K)=	-336.007845	G3 Energy=	-335.998427
G3 Enthalpy=	-335.997483	G3 Free Energy=	-336.043181

For Anharmonic Corrections of 3a-6

Vibrational temperatures: 60.41 75.34 146.96 207.27 378.34
(Kelvin) 437.85 484.70 599.98 723.42 766.50
851.88 915.96 1030.70 1076.81 1135.13
1207.28 1220.56 1239.46 1323.60 1386.53
1421.12 1428.50 1465.01 1514.74 1522.94

1524.00 1600.66 1676.25 1715.11 1746.01
1775.60 1789.02 1860.23 1891.18 1959.22
1974.64 1989.36 2078.59 2160.99 2188.07
2224.56 2364.74 2396.02 3741.98 3844.39
4256.49 4358.54 4380.67 4436.55 4560.06
4561.68 4582.53 4595.56 4614.25

Zero-point correction= 0.166999 (Hartree/Particle)
Thermal correction to Energy= 0.176125
Thermal correction to Enthalpy= 0.177069
Thermal correction to Gibbs Free Energy= 0.131923
Sum of electronic and zero-point Energies= -336.140869
Sum of electronic and thermal Energies= -336.131743
Sum of electronic and thermal Enthalpies= -336.130799
Sum of electronic and thermal Free Energies= -336.175945

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	110.520	33.845	95.018

ZPE(harm) = 0.43846D+03 kJ/mol ZPE(anh)= 0.43187D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.82752D-74	0.95177D-73	
QZvib	0.53915D+03	0.43559D+03	
Energy	0.46242D+03	0.45442D+03	kJ/mol
Enthalpy	0.46490D+03	0.45690D+03	kJ/mol
Entropy	0.39755D+03	0.39936D+03	J/(mol K)
Sp.Heat(V)	0.14161D+03	0.13574D+03	J/(mol K)
Sp.Heat(P)	0.14992D+03	0.14406D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.82752D-74	0.95177D-73	
QZvib	0.53915D+03	0.43559D+03	
Energy	0.46242D+03	0.45442D+03	kJ/mol
Enthalpy	0.46490D+03	0.45690D+03	kJ/mol
Entropy	0.39755D+03	0.39936D+03	J/(mol K)
Sp.Heat(V)	0.14161D+03	0.13574D+03	J/(mol K)
Sp.Heat(P)	0.14992D+03	0.14406D+03	J/(mol K)

3a-7 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -336.335936920

Zero-point correction= 0.167306 (Hartree/Particle)
Thermal correction to Energy= 0.176084
Thermal correction to Enthalpy= 0.177028
Thermal correction to Gibbs Free Energy= 0.133811
Sum of electronic and ZPE= -336.168631
Sum of electronic and thermal Energies= -336.159853
Sum of electronic and thermal Enthalpies= -336.158909
Sum of electronic and thermal Free Energies= -336.202126

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.494	34.001	90.958

C,0,0.2139030192,-0.2164606455,-0.0070564824
C,0,1.7040579882,-0.5485291475,0.1320767065
C,0,2.6476661623,0.2851641202,-0.7452313257
B,0,1.7061036172,-0.2714328062,1.6762986798
H,0,1.8225091398,-1.6124531334,-0.1005367841
H,0,2.6365440939,1.3449562654,-0.4716992559
H,0,2.3911568665,0.2047070246,-1.8084322349
H,0,3.6784645652,-0.063914885,-0.6208026406
H,0,1.3938295303,-1.1248373546,2.4523896442
H,0,1.9370317801,0.8321820741,2.0786642336
C,0,-0.7495501804,-1.2402097647,0.0902045694
C,0,-2.1119901453,-0.9602519069,-0.0038037306
C,0,-2.5472910413,0.3570528526,-0.1827522216
C,0,-1.607906364,1.3872502894,-0.2623918818
C,0,-0.2427582301,1.1057060346,-0.1675108488
H,0,-0.4179750863,-2.2660906964,0.2286353544
H,0,-2.8342342686,-1.7691472649,0.0604521029
H,0,-3.6082353685,0.5769096546,-0.2580983978
H,0,-1.9357580562,2.4141069792,-0.3972456131
H,0,0.4727219781,1.9188523102,-0.2327098735

B3LYP/6-31G*
E(RB+HF-LYP) = -336.309062386

Zero-point correction= 0.168171 (Hartree/Particle)
Thermal correction to Energy= 0.176896
Thermal correction to Enthalpy= 0.177840

Thermal correction to Gibbs Free Energy= 0.134727
Sum of electronic and ZPE= -336.140892
Sum of electronic and thermal Energies= -336.132166
Sum of electronic and thermal Enthalpies= -336.131222
Sum of electronic and thermal Free Energies= -336.174335

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.004	33.811	90.740

C,0,0.2181025627,-0.2173538408,-0.0108418883
C,0,1.7092164621,-0.5478481114,0.1248524289
C,0,2.6499810578,0.2933902041,-0.7460450531
B,0,1.6863503057,-0.2709043595,1.6679032644
H,0,1.8320659334,-1.6106467164,-0.1117689233
H,0,2.6417511091,1.3505322234,-0.4598126983
H,0,2.3901596679,0.2269953699,-1.8099688797
H,0,3.6812239689,-0.0586981654,-0.62947714
H,0,1.3713776072,-1.1276056688,2.4411303562
H,0,1.8986110684,0.8357350905,2.07501798
C,0,-0.7426783479,-1.240695089,0.1023457749
C,0,-2.1041963356,-0.9636985389,0.0127084184
C,0,-2.5410494101,0.3501624381,-0.175814601
C,0,-1.6049499383,1.3804389451,-0.268512169
C,0,-0.2407405551,1.1022337251,-0.1778975957
H,0,-0.4074654732,-2.2646821467,0.2488150622
H,0,-2.8255447249,-1.7730510562,0.0883936726
H,0,-3.6031953163,0.5680707695,-0.2477112681
H,0,-1.9354351609,2.4060470556,-0.4101578889
H,0,0.4747055192,1.9151378717,-0.2527088522

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.161444	E(Thermal)=	0.170477
E(QCISD(T))=	-335.230618	E(Empiric)=	-0.155480
DE(Plus)=	-0.019444	DE(2DF)=	-0.284782
E(Delta-G3)=	-0.480918	E(G3-Empiric)=	-0.155480
G3(0 K)=	-336.009799	G3 Energy=	-336.000766
G3 Enthalpy=	-335.999822	G3 Free Energy=	-336.043489

For Anharmonic Corrections of 3a-7

Vibrational temperatures: 73.44 170.12 290.24 340.71 347.06
(Kelvin) 451.05 564.33 596.61 624.48 735.36
790.03 910.75 1019.21 1073.08 1105.96
1165.76 1235.22 1285.38 1338.09 1394.55

1414.07 1434.80 1462.14 1496.53 1529.36
1563.48 1587.97 1637.05 1699.71 1718.07
1738.99 1753.49 1812.55 1930.71 1968.76
2004.86 2074.66 2153.61 2196.17 2204.40
2217.00 2351.75 2382.14 3750.99 3863.81
4379.58 4406.73 4470.54 4485.71 4576.62
4586.64 4600.45 4615.72 4626.79

Zero-point correction= 0.168169 (Hartree/Particle)
Thermal correction to Energy= 0.176895
Thermal correction to Enthalpy= 0.177839
Thermal correction to Gibbs Free Energy= 0.134725
Sum of electronic and zero-point Energies= -336.140893
Sum of electronic and thermal Energies= -336.132167
Sum of electronic and thermal Enthalpies= -336.131223
Sum of electronic and thermal Free Energies= -336.174337

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.003	33.811	90.741

ZPE(harm) = 0.44153D+03 kJ/mol ZPE(anh)= 0.43539D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.49670D-75	0.91434D-74	
QZvib	0.11182D+03	0.17309D+03	
Energy	0.46444D+03	0.45908D+03	kJ/mol
Enthalpy	0.46692D+03	0.46156D+03	kJ/mol
Entropy	0.37966D+03	0.38590D+03	J/(mol K)
Sp.Heat(V)	0.14147D+03	0.14478D+03	J/(mol K)
Sp.Heat(P)	0.14978D+03	0.15310D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.49670D-75	0.91434D-74	
QZvib	0.11182D+03	0.17309D+03	
Energy	0.46444D+03	0.45908D+03	kJ/mol
Enthalpy	0.46692D+03	0.46156D+03	kJ/mol
Entropy	0.37966D+03	0.38590D+03	J/(mol K)
Sp.Heat(V)	0.14147D+03	0.14478D+03	J/(mol K)
Sp.Heat(P)	0.14978D+03	0.15310D+03	J/(mol K)

A. 3. Theoretical Structures from "Dynamics and Slectivity In The Hydroboration Of Internal Disubstituted and Trisubstituted Alkenes"

4a-1

B3LYP/6-31G**
E(RB+HF-LYP) = -157.244953821

Zero-point correction= 0.107744 (Hartree/Particle)
Thermal correction to Energy= 0.113227
Thermal correction to Enthalpy= 0.114171
Thermal correction to Gibbs Free Energy= 0.080339
Sum of electronic and ZPE= -157.137210
Sum of electronic and thermal Energies= -157.131727
Sum of electronic and thermal Enthalpies= -157.130783
Sum of electronic and thermal Free Energies= -157.164614

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	71.051	18.324	71.205

C,0,-0.0741869005,-0.0656741993,0.02700068
C,0,0.0558360362,0.1720604324,1.3373723039
H,0,0.8027112934,-0.3983584949,-0.5322842797
C,0,1.3261226161,0.0194559041,2.126625228
H,0,-0.8210430436,0.5048203564,1.8966328668
C,0,-1.3444856286,0.0866871987,-0.7622588185
H,0,-2.1722467894,0.422727841,-0.1291788494
H,0,-1.2227615999,0.813678887,-1.5756760765
H,0,-1.6384756414,-0.861907084,-1.2299105154
H,0,1.2044666566,-0.7085421964,2.9391749926
H,0,2.1540415975,-0.3157612291,1.4933064998
H,0,1.6198164037,0.9675805841,2.5953389684

B3LYP/6-31G*
E(RB+HF-LYP) = -157.226915627

Zero-point correction= 0.108534 (Hartree/Particle)
Thermal correction to Energy= 0.113989
Thermal correction to Enthalpy= 0.114933
Thermal correction to Gibbs Free Energy= 0.081158
Sum of electronic and ZPE= -157.118381
Sum of electronic and thermal Energies= -157.112927

Sum of electronic and thermal Enthalpies= -157.111983
Sum of electronic and thermal Free Energies= -157.145757

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	71.529	18.175	71.085

C,0,-0.0732372391,-0.0658515462,0.0283746778
C,0,0.0548401811,0.1719074774,1.3362290065
H,0,0.8033259451,-0.3985088392,-0.5316957024
C,0,1.3242770442,0.0202433479,2.1252877668
H,0,-0.8218915423,0.5042709337,1.8962185704
C,0,-1.3426563613,0.0858733608,-0.7609068214
H,0,-2.1716954343,0.4212079177,-0.1281300085
H,0,-1.222772731,0.813600237,-1.5752754356
H,0,-1.6376967245,-0.862546617,-1.2305048064
H,0,1.2050251592,-0.7076391967,2.9395514234
H,0,2.1532013984,-0.3145623849,1.4920841862
H,0,1.6190753046,0.9687733096,2.5949101433

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.104193	E(Thermal)=	0.109780
E(QCISD(T))=	-156.694162	E(Empiric)=	-0.081120
DE(Plus)=	-0.008648	DE(2DF)=	-0.155598
E(Delta-G3)=	-0.224926	E(G3-Empiric)=	-0.081120
G3(0 K)=	-157.060262	G3 Energy=	-157.054674
G3 Enthalpy=	-157.053730	G3 Free Energy=	-157.087748

For Anharmonic Corrections of 4a-1

Zero-point vibrational energy 283735.3 (Joules/Mol)
67.81437 (Kcal/Mol)
Vibrational temperatures: 279.53 359.35 392.67 714.43 1082.07
(Kelvin) 1281.33 1445.49 1460.82 1527.07 1548.12
1553.10 1678.38 1927.18 1942.95 2069.02
2071.88 2170.96 2186.35 2191.88 2193.14
2513.74 4367.23 4386.13 4434.48 4459.91
4481.52 4496.48 4506.45 4529.32

Zero-point correction= 0.108069 (Hartree/Particle)
Thermal correction to Energy= 0.113014
Thermal correction to Enthalpy= 0.113958
Thermal correction to Gibbs Free Energy= 0.081075
Sum of electronic and zero-point Energies= -157.115551

Sum of electronic and thermal Energies= -157.110606
Sum of electronic and thermal Enthalpies= -157.109662
Sum of electronic and thermal Free Energies= -157.142546

E (Thermal)	CV	S	
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	70.917	16.426	69.209

ZPE(harm) = 0.28242D+03 kJ/mol ZPE(anh)= 0.27825D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.12791D-48	0.70659D-48	
QZvib	0.38374D+01	0.39536D+01	
Energy	0.29540D+03	0.29133D+03	kJ/mol
Enthalpy	0.29788D+03	0.29380D+03	kJ/mol
Entropy	0.29788D+03	0.29843D+03	J/(mol K)
Sp.Heat(V)	0.68728D+02	0.69717D+02	J/(mol K)
Sp.Heat(P)	0.77043D+02	0.78031D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.12791D-48	0.70659D-48	
QZvib	0.38374D+01	0.39536D+01	
Energy	0.29540D+03	0.29133D+03	kJ/mol
Enthalpy	0.29788D+03	0.29380D+03	kJ/mol
Entropy	0.29788D+03	0.29843D+03	J/(mol K)
Sp.Heat(V)	0.68728D+02	0.69717D+02	J/(mol K)
Sp.Heat(P)	0.77043D+02	0.78031D+02	J/(mol K)

4a-2 Complex
B3LYP/6-31+G**
E(RB+HF-LYP) = -183.877535121

Zero-point correction= 0.140052 (Hartree/Particle)
Thermal correction to Energy= 0.147554
Thermal correction to Enthalpy= 0.148499
Thermal correction to Gibbs Free Energy= 0.109828
Sum of electronic and ZPE= -183.737483
Sum of electronic and thermal Energies= -183.729981
Sum of electronic and thermal Enthalpies= -183.729037
Sum of electronic and thermal Free Energies= -183.767707

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	92.592	26.832	81.390

H,0,0.0902548938,-0.260295644,0.06965851
C,0,0.0733633837,-0.1460612448,1.1520867413
C,0,1.2664353628,0.094376231,1.7817605338
B,0,0.2940611422,1.7966318755,1.5146275954
C,0,-1.1974153485,-0.569463766,1.8377390408
C,0,2.6062941971,0.0632297055,1.0928294304
H,0,1.2836042078,0.0628030964,2.8696165873
H,0,-0.204621251,1.9908766547,2.5875920917
H,0,-0.4574919546,1.9056789373,0.5759514898
H,0,1.334810157,2.3412266939,1.2670833596
H,0,3.0613297127,-0.9270003238,1.2262606612
H,0,2.5092689231,0.252273809,0.0198934189
H,0,3.2895407957,0.806141816,1.512253749
H,0,-2.0664948935,-0.0512040889,1.4231861109
H,0,-1.3437765125,-1.6465170084,1.6850587372
H,0,-1.1580698158,-0.3756117434,2.9124199427

B3LYP/6-31G*
E(RB+HF-LYP) = -183.857602343

Zero-point correction= 0.141068 (Hartree/Particle)
Thermal correction to Energy= 0.148552
Thermal correction to Enthalpy= 0.149496
Thermal correction to Gibbs Free Energy= 0.110811
Sum of electronic and ZPE= -183.716534
Sum of electronic and thermal Energies= -183.709050
Sum of electronic and thermal Enthalpies= -183.708106
Sum of electronic and thermal Free Energies= -183.746791

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	93.218	26.640	81.420

Zero-point correction= 0.141068 (Hartree/Particle)
Thermal correction to Energy= 0.148552
Thermal correction to Enthalpy= 0.149496
Thermal correction to Gibbs Free Energy= 0.110811
Sum of electronic and ZPE= -183.716534
Sum of electronic and thermal Energies= -183.709050
Sum of electronic and thermal Enthalpies= -183.708106
Sum of electronic and thermal Free Energies= -183.746791

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	93.218	26.640	81.420

H,0,0.0914673942,-0.2666236287,0.071233912
C,0,0.0747688786,-0.1490709583,1.1534885507
C,0,1.2674686267,0.0914218198,1.7814525139
B,0,0.2896108371,1.7962986915,1.5126075862
C,0,-1.1965712439,-0.5685784059,1.8400300475
C,0,2.6060473225,0.0644178344,1.0907646908
H,0,1.2865511077,0.0618815602,2.869477809
H,0,-0.2199382122,1.983798061,2.5821400924
H,0,-0.4473105204,1.910813901,0.5624980488
H,0,1.3370460408,2.3400930546,1.2858849782
H,0,3.0704477784,-0.9213782138,1.2308485499
H,0,2.505567983,0.2435836808,0.0159264307
H,0,3.284722352,0.8162517005,1.5029003086
H,0,-2.0630299113,-0.0399987249,1.4317737435
H,0,-1.353404282,-1.6439647745,1.6807264264
H,0,-1.1523511512,-0.381860598,2.9162643115

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.135426	E(Thermal)=	0.143125
E(QCISD(T))=	-183.198386	E(Empiric)=	-0.101400
DE(Plus)=	-0.009181	DE(2DF)=	-0.197756
E(Delta-G3)=	-0.273804	E(G3-Empiric)=	-0.101400
G3(0 K)=	-183.645101	G3 Energy=	-183.637402
G3 Enthalpy=	-183.636458	G3 Free Energy=	-183.675553

For Anharmonic Corrections of 4a-2

Zero-point vibrational energy 370153.6 (Joules/Mol)
88.46884 (Kcal/Mol)
Vibrational temperatures: 53.63 285.62 309.22 377.51 414.77
(Kelvin) 419.68 446.65 637.02 703.33 1064.55
1189.48 1265.79 1275.56 1439.83 1499.29
1534.38 1562.59 1589.28 1613.70 1686.21
1705.25 1723.35 1920.70 1941.83 2075.57
2077.56 2168.26 2174.00 2185.12 2193.08
2386.11 3628.17 3718.07 3800.37 4388.28
4393.79 4487.28 4492.11 4529.72 4536.51
4564.88 4580.30

Zero-point correction= 0.140984 (Hartree/Particle)
Thermal correction to Energy= 0.148584
Thermal correction to Enthalpy= 0.149528
Thermal correction to Gibbs Free Energy= 0.110086
Sum of electronic and zero-point Energies= -183.716609
Sum of electronic and thermal Energies= -183.709009
Sum of electronic and thermal Enthalpies= -183.708065
Sum of electronic and thermal Free Energies= -183.747507

E (Thermal)	CV	S	
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	93.238	26.711	83.013

ZPE(harm) = 0.37015D+03 kJ/mol ZPE(anh)= 0.36506D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.97524D-63	0.29439D-62	
QZvib	0.68730D+02	0.26554D+02	
Energy	0.39011D+03	0.38507D+03	kJ/mol
Enthalpy	0.39259D+03	0.38755D+03	kJ/mol
Entropy	0.34733D+03	0.33963D+03	J/(mol K)
Sp.Heat(V)	0.11176D+03	0.11522D+03	J/(mol K)
Sp.Heat(P)	0.12007D+03	0.12354D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.97524D-63	0.29439D-62	
QZvib	0.68730D+02	0.26554D+02	
Energy	0.39011D+03	0.38507D+03	kJ/mol
Enthalpy	0.39259D+03	0.38755D+03	kJ/mol
Entropy	0.34733D+03	0.33963D+03	J/(mol K)
Sp.Heat(V)	0.11176D+03	0.11522D+03	J/(mol K)
Sp.Heat(P)	0.12007D+03	0.12354D+03	J/(mol K)

4a-3 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -183.875233540

Zero-point correction= 0.139944 (Hartree/Particle)
Thermal correction to Energy= 0.146439

Thermal correction to Enthalpy= 0.147383
Thermal correction to Gibbs Free Energy= 0.111004
Sum of electronic and ZPE= -183.735290
Sum of electronic and thermal Energies= -183.728795
Sum of electronic and thermal Enthalpies= -183.727851
Sum of electronic and thermal Free Energies= -183.764229

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	91.892	24.231	76.565

H,0,0.0547492498,0.2939452218,0.0377869063
C,0,0.0053941434,0.1445387472,1.1154021788
C,0,1.2292419671,0.0810149373,1.8148635859
B,0,0.5609829691,1.6790602787,1.9930973539
C,0,-1.2669349841,-0.4813688221,1.6320145346
C,0,2.5676042967,0.0099037649,1.1042423027
H,0,1.1935479784,-0.4110297902,2.7850368098
H,0,0.1995863625,1.8094329086,3.1279814665
H,0,-0.4738781361,1.7775339743,1.3182640692
H,0,1.3210132285,2.4283479739,1.4507004936
H,0,3.3571584142,0.4711287001,1.7051533308
H,0,2.8538993902,-1.0328092786,0.9149613458
H,0,2.5347386767,0.5339987284,0.1439729115
H,0,-2.1585172275,0.009285175,1.2309459625
H,0,-1.2893733901,-1.5354981829,1.3297049909
H,0,-1.3081199388,-0.4403993366,2.7238897571

B3LYP/6-31G*
E(RB+HF-LYP) = -183.854622951

Zero-point correction= 0.141009 (Hartree/Particle)
Thermal correction to Energy= 0.147448
Thermal correction to Enthalpy= 0.148392
Thermal correction to Gibbs Free Energy= 0.112104
Sum of electronic and ZPE= -183.713614
Sum of electronic and thermal Energies= -183.707175
Sum of electronic and thermal Enthalpies= -183.706231
Sum of electronic and thermal Free Energies= -183.742519

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	92.525	23.948	76.375

H,0,0.0558531105,0.2970083651,0.037700397
C,0,0.0038549411,0.1536080372,1.1163223865
C,0,1.2295461307,0.0892071213,1.8196237067
B,0,0.5711612377,1.6770210179,1.9990013078
C,0,-1.2658323347,-0.4802291007,1.6306634922
C,0,2.5650956384,0.0087275782,1.1049474607
H,0,1.1912072778,-0.4164166023,2.7830805853
H,0,0.1974871917,1.8154410551,3.1292740724
H,0,-0.4696184231,1.7618126422,1.3198960288
H,0,1.3136982899,2.4368880367,1.4455501948
H,0,3.3601144495,0.4640929356,1.7042097655
H,0,2.8462739486,-1.0354336873,0.9118356685
H,0,2.533286238,0.5349648573,0.1451415965
H,0,-2.1609444094,0.0025192902,1.2262653875
H,0,-1.2805211788,-1.5360032516,1.3316532166
H,0,-1.309569108,-0.436123295,2.7228527331

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.135369	E(Thermal)=	0.142015
E(QCISD(T))=	-183.195406	E(Empiric)=	-0.101400
DE(Plus)=	-0.009497	DE(2DF)=	-0.198608
E(Delta-G3)=	-0.273074	E(G3-Empiric)=	-0.101400
G3(0 K)=	-183.642616	G3 Energy=	-183.635970
G3 Enthalpy=	-183.635025	G3 Free Energy=	-183.671672

For Anharmonic Corrections of 4a-3

Zero-point vibrational energy 370221.1 (Joules/Mol)
88.48497 (Kcal/Mol)
Vibrational temperatures: 311.72 324.72 338.91 423.46 437.86
(Kelvin) 612.43 746.72 868.86 1053.44 1177.09
1275.27 1375.80 1445.50 1501.38 1531.82
1570.84 1603.65 1647.67 1675.50 1711.29
1766.28 1863.31 1932.01 2078.90 2081.80
2168.11 2182.72 2190.44 2199.18 2243.58
3359.38 3686.91 3832.50 4372.67 4393.16
4465.49 4487.23 4498.55 4519.62 4540.71
4558.16

Zero-point correction=	0.141010 (Hartree/Particle)
Thermal correction to Energy=	0.147449
Thermal correction to Enthalpy=	0.148393
Thermal correction to Gibbs Free Energy=	0.112105
Sum of electronic and zero-point Energies=	-183.713613

Sum of electronic and thermal Energies= -183.707174
Sum of electronic and thermal Enthalpies= -183.706230
Sum of electronic and thermal Free Energies= -183.742518

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.526	23.948	76.375

ZPE(harm) = 0.36713D+03 kJ/mol ZPE(anh)= 0.36068D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.42222D-63	0.10880D-61	
QZvib	0.87757D+01	0.16805D+02	
Energy	0.38403D+03	0.37871D+03	kJ/mol
Enthalpy	0.38651D+03	0.38119D+03	kJ/mol
Entropy	0.32787D+03	0.33702D+03	J/(mol K)
Sp.Heat(V)	0.10020D+03	0.10401D+03	J/(mol K)
Sp.Heat(P)	0.10851D+03	0.11232D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.42222D-63	0.10880D-61	
QZvib	0.87757D+01	0.16805D+02	
Energy	0.38403D+03	0.37871D+03	kJ/mol
Enthalpy	0.38651D+03	0.38119D+03	kJ/mol
Entropy	0.32787D+03	0.33702D+03	J/(mol K)
Sp.Heat(V)	0.10020D+03	0.10401D+03	J/(mol K)
Sp.Heat(P)	0.10851D+03	0.11232D+03	J/(mol K)

4a-4 Variational Transition State

B3LYP/6-31+G**
E(RB+HF-LYP) = -183.864473782

Zero-point correction= 0.135422 (Hartree/Particle)
Thermal correction to Energy= 0.144431
Thermal correction to Enthalpy= 0.145375
Thermal correction to Gibbs Free Energy= 0.101539
Sum of electronic and zero-point Energies= -183.729051
Sum of electronic and thermal Energies= -183.720043
Sum of electronic and thermal Enthalpies= -183.719099
Sum of electronic and thermal Free Energies= -183.762935

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.632	28.472	92.260

B3LYP/6-31G*
E(RB+HF-LYP) = -183.843394549

Zero-point correction= 0.136202 (Hartree/Particle)
Thermal correction to Energy= 0.144463
Thermal correction to Enthalpy= 0.145407
Thermal correction to Gibbs Free Energy= 0.103314
Sum of electronic and ZPE= -183.707193
Sum of electronic and thermal Energies= -183.698932
Sum of electronic and thermal Enthalpies= -183.697988
Sum of electronic and thermal Free Energies= -183.740080

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	90.652	26.416	88.591

C,0,0.35916,2.01568,-0.0431
C,0,0.51562,0.59078,0.40893
C,0,0.8315,-0.4404,-0.38492
C,0,1.06097,-1.853,0.07235
B,0,-2.77666,-0.31553,-0.0548
H,0,0.3944,0.4088,1.47873
H,0,0.96784,-0.2535,-1.45219
H,0,-2.85694,0.3421,-1.0481
H,0,-2.8394,0.21024,1.01572
H,0,-2.688,-1.50385,-0.13041
H,0,2.08951,-2.17308,-0.14398
H,0,0.89323,-1.95986,1.14946
H,0,0.39741,-2.55676,-0.44679
H,0,-0.63154,2.41342,0.212
H,0,1.09549,2.66626,0.4485
H,0,0.49457,2.11056,-1.12581

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.130754	E(Thermal)=	0.139193
E(QCISD(T))=	-183.183350	E(Empiric)=	-0.101400
DE(Plus)=	-0.010117	DE(2DF)=	-0.194193
E(Delta-G3)=	-0.273565	E(G3-Empiric)=	-0.101400
G3(0 K)=	-183.631871	G3 Energy=	-183.623432
G3 Enthalpy=	-183.622488	G3 Free Energy=	-183.664984

4a-5 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -183.882698369

Zero-point correction= 0.141795 (Hartree/Particle)
Thermal correction to Energy= 0.149245
Thermal correction to Enthalpy= 0.150190
Thermal correction to Gibbs Free Energy= 0.111522
Sum of electronic and ZPE= -183.760779
Sum of electronic and thermal Energies= -183.753329
Sum of electronic and thermal Enthalpies= -183.752385
Sum of electronic and thermal Free Energies= -183.791053

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	93.653	25.989	81.384

Zero-point correction= 0.142841 (Hartree/Particle)
Thermal correction to Energy= 0.150317
Thermal correction to Enthalpy= 0.151261
Thermal correction to Gibbs Free Energy= 0.112487
Sum of electronic and ZPE= -183.739858
Sum of electronic and thermal Energies= -183.732382
Sum of electronic and thermal Enthalpies= -183.731437
Sum of electronic and thermal Free Energies= -183.770211

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.325	25.872	81.607

C,0,1.2734905626,0.1895864374,1.9656622492
C,0,-0.007990071,0.1827103774,1.1135221513
B,0,-0.8860639094,1.4763485916,1.1880669163
H,0,-2.0525531039,1.4438972031,0.9178096732
C,0,0.3307211705,0.0743671536,-0.4065733409
H,0,-0.3870402244,2.5419991243,1.4215309096
H,0,1.8808529551,1.064128177,1.6935694676
H,0,1.8814391085,-0.6944677267,1.7238184186
H,0,-0.6021123407,-0.7082943115,1.3666824778
C,0,0.9971781981,0.2125295431,3.4740559393
H,0,0.9128920907,0.9362396245,-0.7546245783
H,0,0.9369105318,-0.821400537,-0.5877137967
H,0,-0.567435915,-0.0018211276,-1.0288963732
H,0,1.9275128784,0.2009281503,4.0522792498
H,0,0.4406541816,1.112489551,3.7637701692

H,0,0.4041888872,-0.6576062306,3.7810324672

B3LYP/6-31G*
E(RB+HF-LYP) = -183.882706024

Zero-point correction= 0.142876 (Hartree/Particle)
Thermal correction to Energy= 0.150296
Thermal correction to Enthalpy= 0.151240
Thermal correction to Gibbs Free Energy= 0.112625
Sum of electronic and ZPE= -183.739830
Sum of electronic and thermal Energies= -183.732410
Sum of electronic and thermal Enthalpies= -183.731466
Sum of electronic and thermal Free Energies= -183.770081

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.312	25.798	81.272

Zero-point correction= 0.142876 (Hartree/Particle)
Thermal correction to Energy= 0.150296
Thermal correction to Enthalpy= 0.151240
Thermal correction to Gibbs Free Energy= 0.112625
Sum of electronic and ZPE= -183.739830
Sum of electronic and thermal Energies= -183.732410
Sum of electronic and thermal Enthalpies= -183.731466
Sum of electronic and thermal Free Energies= -183.770081

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.312	25.798	81.272

C,0,1.2733318326,0.1903075089,1.965360544
C,0,-0.0079694559,0.1826677514,1.1132371074
B,0,-0.8843611448,1.4778178933,1.1888160576
H,0,-2.0559400995,1.4455570329,0.9374247418
C,0,0.3331651318,0.0727651178,-0.4051456059
H,0,-0.3815930502,2.5465124695,1.4034081625
H,0,1.8799129014,1.066383616,1.6953282833
H,0,1.8837368488,-0.6924331132,1.7228545793
H,0,-0.6012927092,-0.7089056246,1.3668483062
C,0,0.9941369899,0.2111914285,3.4722521261
H,0,0.9167274105,0.9342232702,-0.7531322786
H,0,0.9380992271,-0.8244778586,-0.586063191
H,0,-0.5648817131,-0.0010548308,-1.029015198
H,0,1.9236590762,0.2008866716,4.0528079214

H,0,0.4345841754,1.1103258006,3.7611534054
H,0,0.4013295791,-0.6601331335,3.7778570384

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.137161	E(Thermal)=	0.144783
E(QCISD(T))=	-183.224417	E(Empiric)=	-0.101400
DE(Plus)=	-0.008514	DE(2DF)=	-0.197545
E(Delta-G3)=	-0.273296	E(G3-Empiric)=	-0.101400
G3(0 K)=	-183.668012	G3 Energy=	-183.660389
G3 Enthalpy=	-183.659445	G3 Free Energy=	-183.698454

BH_3

B3LYP/6-31G*
E(RB+HF-LYP) = -26.6130001305

Zero-point correction= 0.026496
Thermal correction to Energy= 0.029380
Thermal correction to Enthalpy= 0.030324
Thermal correction to Gibbs Free Energy= 0.008941
Sum of electronic and ZPE= -26.586504
Sum of electronic and thermal Energies= -26.583620
Sum of electronic and thermal Enthalpies= -26.582676
Sum of electronic and thermal Free Energies= -26.604059

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	18.436	6.588	45.005

B,0,0.,0.,0.
H,0,0.,0.,1.1939603125
H,0,1.0339999617,0.,-0.5969801563
H,0,-1.0339999618,0.,-0.5969801562

4b-1 Starting Material
B3LYP/6-31G*
E(RB+HF-LYP) = -235.852832184

Zero-point correction= 0.163682 (Hartree/Particle)
Thermal correction to Energy= 0.170163

Thermal correction to Enthalpy= 0.171107
Thermal correction to Gibbs Free Energy= 0.133751
Sum of electronic and ZPE= -235.689150
Sum of electronic and thermal Energies= -235.682669
Sum of electronic and thermal Enthalpies= -235.681725
Sum of electronic and thermal Free Energies= -235.719081

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	106.779	23.695	78.623

C,0,-0.0223375128,0.,0.0065334588
C,0,-0.0200865773,0.,1.3533483743
C,0,1.2728354737,0.,-0.7824807793
C,0,1.2920469385,0.,2.1169171108
C,0,-1.3002651802,0.,2.1741280999
C,0,-1.2814269255,0.,-0.8258728517
H,0,-2.194791071,0.,-0.2267016692
H,0,-1.3145277907,0.8792695565,-1.4856265904
H,0,-1.3145277907,-0.8792695565,-1.4856265904
H,0,1.0830322553,0.,-1.8609888363
H,0,1.8915927527,0.88018288,-0.5593930131
H,0,1.8915927527,-0.88018288,-0.5593930131
H,0,-1.0811261081,0.,3.2462071406
H,0,-1.9233014816,0.8813953612,1.9740809595
H,0,-1.9233014816,-0.8813953612,1.9740809595
H,0,1.1309750504,0.,3.1990341729
H,0,1.9068088689,-0.8792488398,1.8783765338
H,0,1.9068088689,0.8792488398,1.8783765338

4b-2 Complex
B3LYP/6-31G*
E(RB+HF-LYP) = -262.486462233

Zero-point correction= 0.197396 (Hartree/Particle)
Thermal correction to Energy= 0.207819
Thermal correction to Enthalpy= 0.208763
Thermal correction to Gibbs Free Energy= 0.163662
Sum of electronic and ZPE= -262.289066
Sum of electronic and thermal Energies= -262.278644
Sum of electronic and thermal Enthalpies= -262.277699
Sum of electronic and thermal Free Energies= -262.322800

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 130.408 38.168 94.922

C,0,-0.182397631,-0.2567858645,-0.2851082557
C,0,-0.0074120542,-0.171870933,1.2175430822
C,0,1.2169482603,-0.0441061476,1.8434284608
B,0,0.3808069937,1.8075208333,1.5765644026
C,0,-1.2521198406,-0.6155711489,1.9653311372
C,0,2.5383703382,0.0277485503,1.1057953637
C,0,1.4009231832,-0.3381144432,3.3215301808
H,0,-0.8109152555,1.9375188154,1.6824700311
H,0,0.8687487824,2.177996613,0.5457342092
H,0,0.956062318,2.1222982961,2.5855670886
H,0,3.0474093752,-0.9425749222,1.1935803879
H,0,2.4428867477,0.2679024942,0.0477384274
H,0,3.1880457848,0.7798120263,1.5646144831
H,0,-2.1497178769,-0.2223128961,1.4789586381
H,0,-1.3170495847,-1.7127704641,1.9447520431
H,0,-1.2720770382,-0.2971533855,3.007774411
H,0,-1.0470790936,0.3360854756,-0.5997727044
H,0,0.6824498135,0.0850451153,-0.8520914701
H,0,-0.3833998722,-1.3016817651,-0.5609754927
H,0,2.2405572856,0.2368962895,3.7231399688
H,0,0.5222591412,-0.1094703109,3.9249524966
H,0,1.6350822229,-1.4040122278,3.4539911106

4b-3
B3LYP/6-31G*
E(RB+HF-LYP) = -262.483836351

Zero-point correction= 0.197078 (Hartree/Particle)
Thermal correction to Energy= 0.206849
Thermal correction to Enthalpy= 0.207793
Thermal correction to Gibbs Free Energy= 0.164032
Sum of electronic and ZPE= -262.286759
Sum of electronic and thermal Energies= -262.276988
Sum of electronic and thermal Enthalpies= -262.276043
Sum of electronic and thermal Free Energies= -262.319805

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 129.800 36.289 92.103

C,0,-0.1392971075,-0.208802413,-0.3092810773
C,0,-0.0058118395,-0.169900847,1.2000398867
C,0,1.2142374285,-0.0885691486,1.8374627896
B,0,0.3711049724,1.8250386415,1.6468687292
C,0,-1.2755225328,-0.6060106955,1.9066801296
C,0,2.5306002318,-0.0327495927,1.0711038157
C,0,1.3832753909,-0.3762657489,3.3162508796
H,0,-0.771838879,1.9542516538,1.9928110057
H,0,0.6769370774,2.199443994,0.5491370886
H,0,1.156894927,2.1014139472,2.5149284463
H,0,3.3385562669,-0.4237810728,1.6971395049
H,0,2.5017955279,-0.6305223099,0.1558729325
H,0,2.7951859178,0.9923467737,0.7957394518
H,0,-2.148327734,-0.1173145416,1.463499237
H,0,-1.4040442657,-1.6905459524,1.7792251667
H,0,-1.2788043426,-0.3900722005,2.9750477822
H,0,-0.9993519212,0.3871289639,-0.6307858479
H,0,0.7393760891,0.1672692826,-0.8326409356
H,0,-0.3214781303,-1.2447537323,-0.6303729231
H,0,2.2159199822,0.2042605218,3.7239789885
H,0,0.4965200593,-0.1488831778,3.9089428835
H,0,1.6224548815,-1.4405823455,3.4538700658

4c-1 Starting Material

B3LYP/6-31+G**
E(RB+HF-LYP) = -196.558237265

Zero-point correction= 0.134943 (Hartree/Particle)
Thermal correction to Energy= 0.140674
Thermal correction to Enthalpy= 0.141618
Thermal correction to Gibbs Free Energy= 0.106107
Sum of electronic and ZPE= -196.423294
Sum of electronic and thermal Energies= -196.417563
Sum of electronic and thermal Enthalpies= -196.416619
Sum of electronic and thermal Free Energies= -196.452130

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	88.274	20.156	74.739

C,0,-0.0497479703,0.,0.0042255851

C,0,-0.019728463,0.,1.3469528012
H,0,0.9046034248,0.,-0.5255040807
C,0,1.3160022246,0.,2.0793860189
C,0,-1.2847575764,0.,2.1903871026
C,0,-1.2701225351,0.,-0.8743892988
H,0,-2.2015750579,0.,-0.3022338758
H,0,-1.2826967744,0.8795109921,-1.5321370114
H,0,-1.2826967744,-0.8795109921,-1.5321370114
H,0,1.1830845154,0.,3.1649741997
H,0,1.9150355163,-0.8822641857,1.8248336789
H,0,1.9150355163,0.8822641857,1.8248336789
H,0,-1.0509243177,0.,3.2583403979
H,0,-1.9072258629,0.8814272838,1.9937439073
H,0,-1.9072258629,-0.8814272838,1.9937439073

B3LYP/6-31G*
E(RB+HF-LYP) = -196.537128461

Zero-point correction= 0.135981 (Hartree/Particle)
Thermal correction to Energy= 0.141676
Thermal correction to Enthalpy= 0.142620
Thermal correction to Gibbs Free Energy= 0.107196
Sum of electronic and ZPE= -196.401148
Sum of electronic and thermal Energies= -196.395452
Sum of electronic and thermal Enthalpies= -196.394508
Sum of electronic and thermal Free Energies= -196.429932

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	88.903	19.961	74.557

C,0,-0.0492334174,0.,0.0061462355
C,0,-0.0201118949,0.,1.346388935
H,0,0.9047460723,0.,-0.5250164736
C,0,1.3153321871,0.,2.0780145919
C,0,-1.2855356818,0.,2.1889857503
C,0,-1.2686490106,0.,-0.872390363
H,0,-2.2002242476,0.,-0.2992154248
H,0,-1.2822636621,0.8797770577,-1.531186549
H,0,-1.2822636621,-0.8797770577,-1.531186549
H,0,1.1841388953,0.,3.164535317
H,0,1.9164185617,-0.8817820814,1.8232204257
H,0,1.9164185617,0.8817820814,1.8232204257
H,0,-1.053146392,0.,3.2580783488

H,0,-1.9092831535,0.8813136138,1.9927126646
H,0,-1.9092831535,-0.8813136138,1.9927126646

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.130541	E(Thermal)=	0.136396
E(QCISD(T))=	-195.873048	E(Empiric)=	-0.101400
DE(Plus)=	-0.010101	DE(2DF)=	-0.195438
E(Delta-G3)=	-0.280812	E(G3-Empiric)=	-0.101400
G3(0 K)=	-196.330258	G3 Energy=	-196.324403
G3 Enthalpy=	-196.323459	G3 Free Energy=	-196.359162

For Anharmonic Corrections of 4c-1

Zero-point vibrational energy 359465.9 (Joules/Mol)
85.91441 (Kcal/Mol)
Vibrational temperatures: 182.52 220.86 270.50 383.95 431.13
(Kelvin) 556.26 656.44 759.31 1114.99 1206.46
1397.06 1413.02 1485.86 1546.95 1555.16
1611.91 1646.78 1796.18 2003.67 2073.72
2075.66 2093.90 2162.52 2177.46 2177.90
2189.64 2199.72 2200.17 2533.46 4348.47
4358.50 4362.68 4410.21 4417.00 4417.91
4488.02 4496.31 4516.10 4529.16

Zero-point correction=	0.136913 (Hartree/Particle)
Thermal correction to Energy=	0.143751
Thermal correction to Enthalpy=	0.144695
Thermal correction to Gibbs Free Energy=	0.107176
Sum of electronic and zero-point Energies=	-196.406674
Sum of electronic and thermal Energies=	-196.399836
Sum of electronic and thermal Enthalpies=	-196.398892
Sum of electronic and thermal Free Energies=	-196.436411

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	90.205	23.631	78.965

ZPE(harm) = 0.35947D+03 kJ/mol ZPE(anh)= 0.35367D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.21264D-61	0.33854D-60	
QZvib	0.20104D+02	0.30847D+02	
Energy	0.37742D+03	0.37222D+03	kJ/mol
Enthalpy	0.37990D+03	0.37470D+03	kJ/mol

Entropy	0.33039D+03	0.33598D+03	J/(mol K)
Sp.Heat(V)	0.98871D+02	0.10123D+03	J/(mol K)
Sp.Heat(P)	0.10719D+03	0.10954D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.21264D-61	0.33854D-60	
QZvib	0.20104D+02	0.30847D+02	
Energy	0.37742D+03	0.37222D+03	kJ/mol
Enthalpy	0.37990D+03	0.37470D+03	kJ/mol
Entropy	0.33039D+03	0.33598D+03	J/(mol K)
Sp.Heat(V)	0.98871D+02	0.10123D+03	J/(mol K)
Sp.Heat(P)	0.10719D+03	0.10954D+03	J/(mol K)

4c-2 Complex

B3LYP/6-31+G**

E(RB+HF-LYP) = -223.197344725

Zero-point correction= 0.167712 (Hartree/Particle)
Thermal correction to Energy= 0.176848
Thermal correction to Enthalpy= 0.177792
Thermal correction to Gibbs Free Energy= 0.134221
Sum of electronic and ZPE= -223.029633
Sum of electronic and thermal Energies= -223.020497
Sum of electronic and thermal Enthalpies= -223.019553
Sum of electronic and thermal Free Energies= -223.063124

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.974	32.674	91.703

C,0,-0.0407035609,0.1625783193,-0.4166437745
C,0,0.0350989578,-0.0205878619,1.0813593285
C,0,1.2191523285,-0.0025431995,1.7859363278
B,0,0.4373963494,1.7944934971,1.9071162207
C,0,-1.2124235562,-0.5799991895,1.730282799
C,0,2.6173637482,0.0835024585,1.2283243051
H,0,1.1702802836,-0.3642488384,2.8103556302
H,0,0.4980337665,1.8469091951,3.1062488802
H,0,-0.6912380001,1.9792412367,1.5272316983
H,0,1.2480811631,2.3879142109,1.2520733795
H,0,3.2573392297,0.6801975029,1.8842546858

H,0,3.0468077162,-0.9257832498,1.1724492478
H,0,2.6523685198,0.5254711117,0.2314658254
H,0,-2.106632831,-0.0340677304,1.4173497261
H,0,-1.3335590066,-1.6278682921,1.4250770831
H,0,-1.1497498016,-0.5482605978,2.8208256774
H,0,-0.9723617852,0.6603855899,-0.698778386
H,0,0.7910269202,0.7452825378,-0.8138155314
H,0,-0.0295164415,-0.824401701,-0.898008123

B3LYP/6-31G*
E(RB+HF-LYP) = -223.174001523

Zero-point correction= 0.168996 (Hartree/Particle)
Thermal correction to Energy= 0.178073
Thermal correction to Enthalpy= 0.179017
Thermal correction to Gibbs Free Energy= 0.135804
Sum of electronic and ZPE= -223.005005
Sum of electronic and thermal Energies= -222.995929
Sum of electronic and thermal Enthalpies= -222.994985
Sum of electronic and thermal Free Energies= -223.038197

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.742	32.413	90.948

C,0,-0.0409795299,0.1628688217,-0.4162929186
C,0,0.0360455897,-0.0221273466,1.0813436996
C,0,1.2191552179,-0.0045673225,1.7853689796
B,0,0.4370753277,1.792373891,1.9048370097
C,0,-1.2118704148,-0.5795660377,1.7310056646
C,0,2.6177754122,0.0842231073,1.2298539351
H,0,1.1706982272,-0.367075997,2.8098546935
H,0,0.4985346323,1.843362765,3.1046846008
H,0,-0.6929539056,1.9800079959,1.5250021736
H,0,1.2482605027,2.3857736358,1.2487886062
H,0,3.2554620028,0.684144804,1.8860469405
H,0,3.0514552919,-0.9241265226,1.1753683222
H,0,2.6523168047,0.5250130247,0.2317544378
H,0,-2.1058925218,-0.0314634989,1.4193881055
H,0,-1.3379216532,-1.6277798986,1.4262019444
H,0,-1.1480392735,-0.5484342479,2.8222135675
H,0,-0.9725836357,0.6625700936,-0.6976848352
H,0,0.791653383,0.7459966174,-0.8130611798
H,0,-0.0314274577,-0.8229788849,-0.901568747

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162252	E(Thermal)=	0.171570
E(QCISD(T))=	-222.384768	E(Empiric)=	-0.121680
DE(Plus)=	-0.011384	DE(2DF)=	-0.237874
E(Delta-G3)=	-0.329576	E(G3-Empiric)=	-0.121680
G3(0 K)=	-222.923031	G3 Energy=	-222.913713
G3 Enthalpy=	-222.912769	G3 Free Energy=	-222.956176

For Anharmonic Corrections of 4c-2

Zero-point vibrational energy 443744.4 (Joules/Mol)
106.05747 (Kcal/Mol)
Vibrational temperatures: 41.84 228.25 276.55 291.93 344.86
(Kelvin) 381.17 411.94 421.62 497.16 570.86
689.84 752.91 1086.43 1137.28 1195.86
1341.47 1386.47 1413.44 1487.86 1557.61
1564.05 1586.59 1625.49 1653.11 1700.93
1712.01 1805.79 2003.87 2068.48 2076.33
2086.80 2157.70 2166.97 2173.67 2175.15
2194.06 2209.24 2376.91 3627.14 3702.43
3783.33 4376.19 4377.89 4384.63 4478.54
4481.77 4486.89 4527.65 4536.50 4553.23
4571.59

Zero-point correction= 0.169013 (Hartree/Particle)
Thermal correction to Energy= 0.178074
Thermal correction to Enthalpy= 0.179018
Thermal correction to Gibbs Free Energy= 0.136102
Sum of electronic and zero-point Energies= -223.004988
Sum of electronic and thermal Energies= -222.995928
Sum of electronic and thermal Enthalpies= -222.994984
Sum of electronic and thermal Free Energies= -223.037899

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.743	32.410	90.324

ZPE(harm) = 0.44374D+03 kJ/mol ZPE(anh)= 0.43578D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value
Qvib	0.49427D-75	0.18593D-74

QZvib	0.27198D+03	0.41155D+02	
Energy	0.46753D+03	0.45764D+03	kJ/mol
Enthalpy	0.47001D+03	0.46012D+03	kJ/mol
Entropy	0.37792D+03	0.36406D+03	J/(mol K)
Sp.Heat(V)	0.13560D+03	0.12936D+03	J/(mol K)
Sp.Heat(P)	0.14392D+03	0.13767D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.49427D-75	0.18593D-74	
QZvib	0.27198D+03	0.41155D+02	
Energy	0.46753D+03	0.45764D+03	kJ/mol
Enthalpy	0.47001D+03	0.46012D+03	kJ/mol
Entropy	0.37792D+03	0.36406D+03	J/(mol K)
Sp.Heat(V)	0.13560D+03	0.12936D+03	J/(mol K)
Sp.Heat(P)	0.14392D+03	0.13767D+03	J/(mol K)

4c-3 Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -223.195043183

Zero-point correction= 0.167915 (Hartree/Particle)
Thermal correction to Energy= 0.175752
Thermal correction to Enthalpy= 0.176696
Thermal correction to Gibbs Free Energy= 0.137301
Sum of electronic and ZPE= -223.027129
Sum of electronic and thermal Energies= -223.019291
Sum of electronic and thermal Enthalpies= -223.018347
Sum of electronic and thermal Free Energies= -223.057742

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.286	29.878	82.913

C,0,-0.0333257075,0.2315654449,-0.353256078
C,0,-0.0013099405,0.1277025249,1.1587516235
C,0,1.2286478086,0.1092232158,1.873100191
B,0,0.5418813386,1.6849605034,2.0547483718
C,0,-1.2150443413,-0.52930877,1.7866116903
C,0,2.5980600406,0.0406501947,1.2209666311
H,0,1.1820133121,-0.3953122343,2.8367076556
H,0,0.2098715047,1.8357459262,3.1967733665

H,0,-0.5254179605,1.7250923536,1.4260103095
H,0,1.2491093712,2.4546126242,1.4667857693
H,0,3.3605207992,0.4201573608,1.9081005098
H,0,2.8633864222,-0.9946737469,0.968400819
H,0,2.6597408646,0.6390961565,0.3092220511
H,0,-2.1493958946,-0.0866386318,1.4277305031
H,0,-1.2154231058,-1.5929043104,1.5163784857
H,0,-1.1881924559,-0.454973305,2.8762937112
H,0,-1.0129380411,0.567464292,-0.705851489
H,0,0.7240414848,0.9171191559,-0.7359435296
H,0,0.1605385005,-0.7613637546,-0.7784255918

B3LYP/6-31G*
E(RB+HF-LYP) = -223.170802726

Zero-point correction= 0.169178 (Hartree/Particle)
Thermal correction to Energy= 0.176953
Thermal correction to Enthalpy= 0.177897
Thermal correction to Gibbs Free Energy= 0.138599
Sum of electronic and ZPE= -223.001625
Sum of electronic and thermal Energies= -222.993850
Sum of electronic and thermal Enthalpies= -222.992905
Sum of electronic and thermal Free Energies= -223.032204

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.040	29.553	82.710

C,0,-0.0330339411,0.2352110421,-0.3523002506
C,0,-0.0038415736,0.1369586092,1.1605136589
C,0,1.2291502027,0.1174798734,1.8777624035
B,0,0.5527469682,1.6822640615,2.0601828428
C,0,-1.2145015794,-0.5277692204,1.7867664615
C,0,2.5958127348,0.0382712041,1.2207437129
H,0,1.1811677364,-0.4005508801,2.8346905399
H,0,0.2029237382,1.8410018016,3.1963438181
H,0,-0.5189608708,1.7073736652,1.4239106445
H,0,1.2412291781,2.462661346,1.4629063036
H,0,3.3639384468,0.4111397197,1.906195256
H,0,2.8551463584,-0.9982174004,0.9638489898
H,0,2.6589540869,0.6386614865,0.3095235626
H,0,-2.1525139922,-0.0951914306,1.4232192061
H,0,-1.2061020812,-1.59319474,1.5216855573
H,0,-1.1913917903,-0.4483695071,2.8768027466

H,0,-1.0128246726,0.5674838162,-0.710064643
H,0,0.7244436157,0.9217423003,-0.7349651564
H,0,0.1644214352,-0.7587407476,-0.7746606541

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162410	E(Thermal)=	0.170448
E(QCISD(T))=	-222.382000	E(Empiric)=	-0.121680
DE(Plus)=	-0.011773	DE(2DF)=	-0.238845
E(Delta-G3)=	-0.328665	E(G3-Empiric)=	-0.121680
G3(0 K)=	-222.920553	G3 Energy=	-222.912515
G3 Enthalpy=	-222.911571	G3 Free Energy=	-222.951338

E(RB+HF-LYP) = -26.6130001305

For Anharmonic Corrections of 4c-3

Zero-point vibrational energy 444034.5 (Joules/Mol)
106.12678 (Kcal/Mol)
Warning -- explicit consideration of 11 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 230.81 263.32 290.62 328.34 406.38
(Kelvin) 439.46 513.24 597.80 684.37 793.05
808.67 1038.68 1158.81 1180.76 1367.80
1385.71 1418.06 1490.70 1548.43 1583.10
1592.37 1611.78 1665.96 1684.87 1708.47
1811.73 1972.96 2062.95 2076.70 2085.77
2146.26 2166.51 2176.53 2182.26 2195.98
2213.87 2242.36 3407.36 3676.88 3819.55
4379.06 4391.66 4399.83 4477.39 4486.09
4493.46 4517.61 4534.71 4543.11 4557.85

Zero-point correction=	0.169124 (Hartree/Particle)		
Thermal correction to Energy=	0.177003		
Thermal correction to Enthalpy=	0.177947		
Thermal correction to Gibbs Free Energy=	0.138404		
Sum of electronic and zero-point Energies=	-223.001715		
Sum of electronic and thermal Energies=	-222.993836		
Sum of electronic and thermal Enthalpies=	-222.992891		
Sum of electronic and thermal Free Energies=	-223.032434		

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	111.071	29.750	83.225

ZPE(harm) = 0.44124D+03 kJ/mol ZPE(anh)= 0.43393D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.13811D-75	0.45000D-74	
QZvib	0.27716D+02	0.47229D+02	
Energy	0.46193D+03	0.45553D+03	kJ/mol
Enthalpy	0.46441D+03	0.45801D+03	kJ/mol
Entropy	0.35653D+03	0.36402D+03	J/(mol K)
Sp.Heat(V)	0.12447D+03	0.12813D+03	J/(mol K)
Sp.Heat(P)	0.13279D+03	0.13644D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.13811D-75	0.45000D-74	
QZvib	0.27716D+02	0.47229D+02	
Energy	0.46193D+03	0.45553D+03	kJ/mol
Enthalpy	0.46441D+03	0.45801D+03	kJ/mol
Entropy	0.35653D+03	0.36402D+03	J/(mol K)
Sp.Heat(V)	0.12447D+03	0.12813D+03	J/(mol K)
Sp.Heat(P)	0.13279D+03	0.13644D+03	J/(mol K)

4c-4 Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -223.190979179

Zero-point correction= 0.168021 (Hartree/Particle)
Thermal correction to Energy= 0.175825
Thermal correction to Enthalpy= 0.176769
Thermal correction to Gibbs Free Energy= 0.137487
Sum of electronic and ZPE= -223.022959
Sum of electronic and thermal Energies= -223.015154
Sum of electronic and thermal Enthalpies= -223.014210
Sum of electronic and thermal Free Energies= -223.053492

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.332	29.822	82.675

H,0,0.0769302656,0.0097752069,0.0756288462
C,0,-0.0066266875,0.0427743338,1.1607434225
C,0,1.2205815994,0.1227775673,1.8782144803

B,0,0.5140890387,1.7028426563,1.7700346314
C,0,-1.2935765288,-0.5319958184,1.7057818235
C,0,2.5183207065,-0.0074893814,1.0867277294
C,0,1.3317434575,-0.4121367483,3.3009860989
H,0,0.1278914355,2.0206087151,2.8580781916
H,0,-0.5246288484,1.6299128265,1.0893562416
H,0,1.2295645441,2.3877650567,1.099004705
H,0,2.8349761323,-1.0585245999,1.0342120946
H,0,2.4106796324,0.3685019143,0.0652151568
H,0,3.3247803146,0.5586421095,1.5642915391
H,0,2.1351417298,0.1044808821,3.8360234149
H,0,0.416650587,-0.276608023,3.8801983551
H,0,1.5773347155,-1.4832847797,3.2916232844
H,0,-2.1528646554,-0.2181393468,1.10611139
H,0,-1.2353981893,-1.6270248464,1.675901426
H,0,-1.4706492495,-0.2314807247,2.7400851686

B3LYP/6-31G*
E(RB+HF-LYP) = -223.167040783

Zero-point correction= 0.169311 (Hartree/Particle)
Thermal correction to Energy= 0.177061
Thermal correction to Enthalpy= 0.178005
Thermal correction to Gibbs Free Energy= 0.138811
Sum of electronic and ZPE= -222.997730
Sum of electronic and thermal Energies= -222.989980
Sum of electronic and thermal Enthalpies= -222.989036
Sum of electronic and thermal Free Energies= -223.028229

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.107	29.524	82.490

H,0,0.076976178,0.0091530232,0.0753750938
C,0,-0.0077681667,0.0483413863,1.1606120698
C,0,1.2214944093,0.1293578179,1.8800432971
B,0,0.5229662626,1.7017245595,1.7751322455
C,0,-1.2934702877,-0.5308614739,1.7053553214
C,0,2.517204921,-0.0075334275,1.087010794
C,0,1.3308690211,-0.4120371363,3.3002028613
H,0,0.1247353041,2.0257657334,2.8577255399
H,0,-0.5197936122,1.6171324399,1.0914141604
H,0,1.2251679131,2.3921585634,1.0942267796
H,0,2.8330574403,-1.0594860355,1.0344666163

H,0,2.4095683155,0.3670419152,0.0641969995
H,0,3.327037173,0.5570647492,1.5619843143
H,0,2.1350896457,0.1008586151,3.8388334554
H,0,0.4149594593,-0.2766956321,3.8797148702
H,0,1.5745509428,-1.4842590656,3.2898810557
H,0,-2.1549280249,-0.2194692049,1.1063612246
H,0,-1.2325885056,-1.6261823788,1.6752580605
H,0,-1.4701883885,-0.2306774485,2.7404232407

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162539	E(Thermal)=	0.170550
E(QCISD(T))=	-222.378385	E(Empiric)=	-0.121680
DE(Plus)=	-0.011474	DE(2DF)=	-0.238875
E(Delta-G3)=	-0.328567	E(G3-Empiric)=	-0.121680
G3(0 K)=	-222.916443	G3 Energy=	-222.908431
G3 Enthalpy=	-222.907487	G3 Free Energy=	-222.947149

4c-5 Variational Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -183.877535121

Zero-point correction= 0.140052 (Hartree/Particle)
Thermal correction to Energy= 0.147554
Thermal correction to Enthalpy= 0.148499
Thermal correction to Gibbs Free Energy= 0.109828
Sum of electronic and ZPE= -183.737483
Sum of electronic and thermal Energies= -183.729981
Sum of electronic and thermal Enthalpies= -183.729037
Sum of electronic and thermal Free Energies= -183.767707

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	92.592	26.832	81.390

H,0,0.0902548938,-0.260295644,0.06965851
C,0,0.0733633837,-0.1460612448,1.1520867413
C,0,1.2664353628,0.094376231,1.7817605338
B,0,0.2940611422,1.7966318755,1.5146275954
C,0,-1.1974153485,-0.569463766,1.8377390408
C,0,2.6062941971,0.0632297055,1.0928294304
H,0,1.2836042078,0.0628030964,2.8696165873
H,0,-0.204621251,1.9908766547,2.5875920917

H,0,-0.4574919546,1.9056789373,0.5759514898
H,0,1.334810157,2.3412266939,1.2670833596
H,0,3.0613297127,-0.9270003238,1.2262606612
H,0,2.5092689231,0.252273809,0.0198934189
H,0,3.2895407957,0.806141816,1.512253749
H,0,-2.0664948935,-0.0512040889,1.4231861109
H,0,-1.3437765125,-1.6465170084,1.6850587372
H,0,-1.1580698158,-0.3756117434,2.9124199427
B3LYP/6-31G*
E(RB+HF-LYP) = -223.160499552

Zero-point correction= 0.164645 (Hartree/Particle)
Thermal correction to Energy= 0.174231
Thermal correction to Enthalpy= 0.175175
Thermal correction to Gibbs Free Energy= 0.130102
Sum of electronic and ZPE= -222.995854
Sum of electronic and thermal Energies= -222.986269
Sum of electronic and thermal Enthalpies= -222.985324
Sum of electronic and thermal Free Energies= -223.030397

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.332	31.823	94.864

C,0,0.79846,-1.76162,-0.64598
C,0,0.66097,-0.40597,0.00701
C,0,0.22311,0.65568,-0.69572
B,0,-2.92834,-0.21737,-0.04186
C,0,1.09688,-0.36338,1.45156
H,0,-0.03215,0.48455,-1.74262
C,0,0.09828,2.08669,-0.24933
H,0,-2.80315,-1.36915,0.24765
H,0,-3.1005,0.09504,-1.18164
H,0,-2.94572,0.61473,0.81433
H,0,0.21059,-2.52258,-0.11505
H,0,0.47259,-1.74753,-1.69065
H,0,1.84361,-2.10156,-0.62001
H,0,0.53281,-1.09332,2.04749
H,0,2.15609,-0.64281,1.5408
H,0,0.96969,0.61745,1.91521
H,0,-0.91128,2.47168,-0.44045
H,0,0.31153,2.22623,0.81375
H,0,0.79014,2.7272,-0.8141

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.158060	E(Thermal)=	0.167876
E(QCISD(T))=	-222.368499	E(Empiric)=	-0.121680
DE(Plus)=	-0.011832	DE(2DF)=	-0.234348
E(Delta-G3)=	-0.329591	E(G3-Empiric)=	-0.121680
G3(0 K)=	-222.907891	G3 Energy=	-222.898075
G3 Enthalpy=	-222.897131	G3 Free Energy=	-222.942715

4c-6 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -223.218920054

Zero-point correction= 0.169597 (Hartree/Particle)
Thermal correction to Energy= 0.178217
Thermal correction to Enthalpy= 0.179161
Thermal correction to Gibbs Free Energy= 0.137806
Sum of electronic and ZPE= -223.049323
Sum of electronic and thermal Energies= -223.040703
Sum of electronic and thermal Enthalpies= -223.039759
Sum of electronic and thermal Free Energies= -223.081114

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.833	31.449	87.038

H,0,1.1232032602,0.3757641274,1.94294744
C,0,0.2820203369,0.2807110418,1.2141998578
B,0,-0.3603713963,1.6778006,1.4852166251
H,0,-1.2368904506,1.8384704313,2.2836149122
C,0,0.9389529861,0.1314052185,-0.1755015887
H,0,0.0884429475,2.6498946364,0.947310918
C,0,-0.5227490586,-0.980313576,1.6376171344
H,0,1.5962393425,0.9786349008,-0.3956736204
H,0,1.5350772733,-0.7871181349,-0.2404013666
H,0,0.187910789,0.089225978,-0.9720266978
H,0,0.0862116242,-1.8563126512,1.3656279929
C,0,-0.7566067388,-1.0457089759,3.1545946784
C,0,-1.8555598841,-1.0945349287,0.8774455799
H,0,-2.3727063199,-2.0273235181,1.1297573064
H,0,-2.5253742571,-0.2651891174,1.1381285479
H,0,-1.71103676,-1.0833500878,-0.2081228527
H,0,-1.2719363163,-1.9731571722,3.4290671347
H,0,0.1908625776,-1.0158060987,3.7059182824

H,0,-1.3732549557,-0.2094656735,3.501983716

B3LYP/6-31G*
E(RB+HF-LYP) = -223.195212165

Zero-point correction= 0.170849 (Hartree/Particle)
Thermal correction to Energy= 0.179450
Thermal correction to Enthalpy= 0.180394
Thermal correction to Gibbs Free Energy= 0.139058
Sum of electronic and ZPE= -223.024363
Sum of electronic and thermal Energies= -223.015762
Sum of electronic and thermal Enthalpies= -223.014818
Sum of electronic and thermal Free Energies= -223.056154

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.607	31.233	86.999

Zero-point correction= 0.170849 (Hartree/Particle)
Thermal correction to Energy= 0.179450
Thermal correction to Enthalpy= 0.180394
Thermal correction to Gibbs Free Energy= 0.139058
Sum of electronic and ZPE= -223.024363
Sum of electronic and thermal Energies= -223.015762
Sum of electronic and thermal Enthalpies= -223.014818
Sum of electronic and thermal Free Energies= -223.056154

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.607	31.233	86.999

H,0,1.1314676279,0.3671135506,1.9414648495
C,0,0.2856088345,0.2789036685,1.2178445637
B,0,-0.3619588946,1.67572153,1.4863327518
H,0,-1.2494188852,1.8361005059,2.2745446209
C,0,0.9355170191,0.1325355771,-0.1749702922
H,0,0.0915387608,2.6506965292,0.9554340715
C,0,-0.5205826269,-0.9816009029,1.6383255732
H,0,1.5894331038,0.9823143801,-0.3982081149
H,0,1.534334166,-0.7845904604,-0.2432139439
H,0,0.1807610266,0.0880893162,-0.9685798641
H,0,0.0877178482,-1.8589263264,1.367522777
C,0,-0.7564253878,-1.044762489,3.1542828988
C,0,-1.8518977372,-1.0937324794,0.8772047373
H,0,-2.3732961587,-2.0240066731,1.1324096277

H,0,-2.5195616731,-0.2604881268,1.132806458
H,0,-1.7055542847,-1.0869060257,-0.2088769919
H,0,-1.2783979398,-1.9689017101,3.4296570635
H,0,0.1911058669,-1.020190738,3.7069734036
H,0,-1.3679556657,-0.2037421258,3.5007498106

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.164018	E(Thermal)=	0.172876
E(QCISD(T))=	-222.406946	E(Empiric)=	-0.121680
DE(Plus)=	-0.010586	DE(2DF)=	-0.237743
E(Delta-G3)=	-0.329081	E(G3-Empiric)=	-0.121680
G3(0 K)=	-222.942018	G3 Energy=	-222.933160
G3 Enthalpy=	-222.932216	G3 Free Energy=	-222.974042

For Anharmonic Corrections of 4c-6

Zero-point vibrational energy 444034.5 (Joules/Mol)
106.12678 (Kcal/Mol)
Vibrational temperatures: 230.81 263.32 290.62 328.34 406.38
(Kelvin) 439.46 513.24 597.80 684.37 793.05
808.67 1038.68 1158.81 1180.76 1367.80
1385.71 1418.06 1490.70 1548.43 1583.10
1592.37 1611.78 1665.96 1684.87 1708.47
1811.73 1972.96 2062.95 2076.70 2085.77
2146.26 2166.51 2176.53 2182.26 2195.98
2213.87 2242.36 3407.36 3676.88 3819.55
4379.06 4391.66 4399.83 4477.39 4486.09
4493.46 4517.61 4534.71 4543.11 4557.85

Zero-point correction=	0.169124 (Hartree/Particle)		
Thermal correction to Energy=	0.177003		
Thermal correction to Enthalpy=	0.177947		
Thermal correction to Gibbs Free Energy=	0.138404		
Sum of electronic and zero-point Energies=	-223.001715		
Sum of electronic and thermal Energies=	-222.993836		
Sum of electronic and thermal Enthalpies=	-222.992891		
Sum of electronic and thermal Free Energies=	-223.032434		

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	111.071	29.750	83.225

ZPE(harm) = 0.44124D+03 kJ/mol ZPE(anh)= 0.43393D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.13811D-75	0.45000D-74	
QZvib	0.27716D+02	0.47229D+02	
Energy	0.46193D+03	0.45553D+03	kJ/mol
Enthalpy	0.46441D+03	0.45801D+03	kJ/mol
Entropy	0.35653D+03	0.36402D+03	J/(mol K)
Sp.Heat(V)	0.12447D+03	0.12813D+03	J/(mol K)
Sp.Heat(P)	0.13279D+03	0.13644D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.13811D-75	0.45000D-74	
QZvib	0.27716D+02	0.47229D+02	
Energy	0.46193D+03	0.45553D+03	kJ/mol
Enthalpy	0.46441D+03	0.45801D+03	kJ/mol
Entropy	0.35653D+03	0.36402D+03	J/(mol K)
Sp.Heat(V)	0.12447D+03	0.12813D+03	J/(mol K)
Sp.Heat(P)	0.13279D+03	0.13644D+03	J/(mol K)

4c-7 Product

B3LYP/6-31+G**

E(RB+HF-LYP) = -223.217898002

Zero-point correction= 0.169770 (Hartree/Particle)
Thermal correction to Energy= 0.178436
Thermal correction to Enthalpy= 0.179380
Thermal correction to Gibbs Free Energy= 0.138174
Sum of electronic and ZPE= -223.048128
Sum of electronic and thermal Energies= -223.039462
Sum of electronic and thermal Enthalpies= -223.038518
Sum of electronic and thermal Free Energies= -223.079724

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.970	31.756	86.727

C,0,1.2222121756,0.2560209797,1.9556362165
C,0,-0.0081874543,0.2143401296,0.9876517231
B,0,-0.6786816807,1.5814807078,1.3573990896
H,0,-1.4645374597,1.6518608504,2.2591982173

C,0,0.5166203282,0.1428525239,-0.4612530365
H,0,-0.3398180204,2.5954310589,0.8167950828
H,0,1.8810322473,1.1088904707,1.7555680219
H,0,1.8170859645,-0.6562245443,1.8127005664
C,0,-0.866769468,-1.0234665843,1.3447022431
H,0,0.9235887823,0.2900362041,3.0098426469
H,0,1.1835797504,0.9837779717,-0.6803739618
H,0,1.0788700793,-0.7859467762,-0.6306743261
H,0,-0.2958030567,0.1744843475,-1.1947940394
H,0,-0.2675299316,-1.9331895409,1.1858870997
H,0,-1.0970018357,-0.9906774832,2.4177979257
C,0,-2.1826267442,-1.1462381401,0.5643746028
H,0,-2.7506592544,-2.0233494916,0.8930475662
H,0,-2.8202303392,-0.2667741075,0.7184677834
H,0,-2.0134080827,-1.2518785762,-0.5123224214

B3LYP/6-31G*
E(RB+HF-LYP) = -223.194425901

Zero-point correction= 0.171028 (Hartree/Particle)
Thermal correction to Energy= 0.179672
Thermal correction to Enthalpy= 0.180616
Thermal correction to Gibbs Free Energy= 0.139435
Sum of electronic and ZPE= -223.023398
Sum of electronic and thermal Energies= -223.014754
Sum of electronic and thermal Enthalpies= -223.013810
Sum of electronic and thermal Free Energies= -223.054991

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

C,0,1.2225669149,0.2538360981,1.9540884507
C,0,-0.0086490005,0.2145155873,0.9882393318
B,0,-0.6805919796,1.5810179106,1.3576367007
H,0,-1.4668236127,1.6525901014,2.2605156663
C,0,0.5157907869,0.1420643055,-0.4600049105
H,0,-0.3436821736,2.596804049,0.8169045693
H,0,1.8820878833,1.1067858497,1.7535486453
H,0,1.8171545064,-0.6592568701,1.8126220034
C,0,-0.866077955,-1.0233595591,1.345405938
H,0,0.9248768164,0.2904126774,3.0091075181
H,0,1.1783355176,0.9863417069,-0.6825963221
H,0,1.0833031316,-0.7842336935,-0.6283837692
H,0,-0.2977140143,0.1673511721,-1.1935768213

H,0,-0.2675776826,-1.9342698979,1.1881536581
H,0,-1.0982729192,-0.9908798814,2.418614575
C,0,-2.1802779893,-1.1444661556,0.5639005251
H,0,-2.7501022208,-2.0217485682,0.890871279
H,0,-2.8168654635,-0.2635461488,0.7179348879
H,0,-2.0097445461,-1.2485286834,-0.5133309254

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.164187	E(Thermal)=	0.173095
E(QCISD(T))=	-222.407158	E(Empiric)=	-0.121680
DE(Plus)=	-0.011077	DE(2DF)=	-0.238051
E(Delta-G3)=	-0.328447	E(G3-Empiric)=	-0.121680
G3(0 K)=	-222.942226	G3 Energy=	-222.933318
G3 Enthalpy=	-222.932373	G3 Free Energy=	-222.974062

For Anharmonic Corrections of 4c-7

Zero-point vibrational energy 444528.5 (Joules/Mol)
106.24487 (Kcal/Mol)
Vibrational temperatures: 250.72 284.39 325.71 367.92 398.86
(Kelvin) 469.19 520.92 549.92 667.94 754.78
870.92 1032.68 1163.37 1199.54 1391.02
1411.30 1463.08 1503.52 1550.93 1556.99
1604.79 1638.55 1652.22 1706.21 1737.74
1819.77 1959.93 2068.20 2074.43 2095.77
2141.80 2171.98 2178.93 2188.33 2201.19
2213.92 2242.78 3333.30 3691.95 3836.97
4356.55 4364.62 4396.58 4454.92 4461.61
4489.28 4498.34 4523.85 4534.93 4555.74

Zero-point correction= 0.169312 (Hartree/Particle)
Thermal correction to Energy= 0.177062
Thermal correction to Enthalpy= 0.178006
Thermal correction to Gibbs Free Energy= 0.138812
Sum of electronic and zero-point Energies= -222.997729
Sum of electronic and thermal Energies= -222.989979
Sum of electronic and thermal Enthalpies= -222.989035
Sum of electronic and thermal Free Energies= -223.028229

E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	111.108	29.524	82.490

ZPE(harm) = 0.44104D+03 kJ/mol ZPE(anh)= 0.43263D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.11986D-75	0.12278D-73	
QZvib	0.22153D+02	0.76183D+02	
Energy	0.46139D+03	0.45488D+03	kJ/mol
Enthalpy	0.46387D+03	0.45736D+03	kJ/mol
Entropy	0.35345D+03	0.37011D+03	J/(mol K)
Sp.Heat(V)	0.12353D+03	0.12882D+03	J/(mol K)
Sp.Heat(P)	0.13184D+03	0.13714D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.11986D-75	0.12278D-73	
QZvib	0.22153D+02	0.76183D+02	
Energy	0.46139D+03	0.45488D+03	kJ/mol
Enthalpy	0.46387D+03	0.45736D+03	kJ/mol
Entropy	0.35345D+03	0.37011D+03	J/(mol K)
Sp.Heat(V)	0.12353D+03	0.12882D+03	J/(mol K)
Sp.Heat(P)	0.13184D+03	0.13714D+03	J/(mol K)

4d-1 Starting Material

B3LYP/6-31+G**

E(RB3LYP) = -273.992565248

Zero-point correction= 0.173685 (Hartree/Particle)
Thermal correction to Energy= 0.180730
Thermal correction to Enthalpy= 0.181674
Thermal correction to Gibbs Free Energy= 0.143064
Sum of electronic and ZPE= -273.818880
Sum of electronic and thermal Energies= -273.811835
Sum of electronic and thermal Enthalpies= -273.810891
Sum of electronic and thermal Free Energies= -273.849501

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.410	27.350	81.262

C,0,0.0325326294,0.0237580912,-0.1924161245
C,0,0.1541154862,-0.1716727253,1.3065247861
C,0,1.3229472598,-0.0026370031,1.9455948957

C,0,-1.1120639378,-0.5548417781,2.0300312448
C,0,2.6112015122,0.4141845925,1.2763080011
H,0,1.3626666187,-0.1722943426,3.0217649747
H,0,3.1184697523,1.1678454303,1.8936559916
H,0,3.2993987351,-0.4452719396,1.2388483101
H,0,-0.585434947,-0.7818272207,-0.6136022231
H,0,-0.5284756479,0.9522591489,-0.3856780398
C,0,1.3915059176,0.0727301095,-0.9073420048
H,0,1.262969358,0.4312398124,-1.9356424355
C,0,2.3806705472,0.9599964376,-0.1412779126
H,0,1.8009945766,-0.9447329928,-0.9761518815
H,0,3.3333295392,1.0339483681,-0.6791576603
H,0,1.9730801229,1.9784396965,-0.0756842406
H,0,-1.9019960727,0.190331206,1.8629144797
H,0,-1.5042433446,-1.5128020344,1.6624744632
H,0,-0.9527141052,-0.6429068565,3.1089773755

B3LYP/6-31G*
E(RB3LYP) = -273.967994363

Zero-point correction= 0.174964 (Hartree/Particle)
Thermal correction to Energy= 0.181968
Thermal correction to Enthalpy= 0.182913
Thermal correction to Gibbs Free Energy= 0.144367
Sum of electronic and ZPE= -273.793030
Sum of electronic and thermal Energies= -273.786026
Sum of electronic and thermal Enthalpies= -273.785082
Sum of electronic and thermal Free Energies= -273.823628

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	114.187	27.079	81.127

C,0,0.0325427257,0.026116347,-0.1931886897
C,0,0.1543247212,-0.1707799041,1.3052354608
C,0,1.3206377974,-0.0026178831,1.9436527977
C,0,-1.1099697407,-0.5560459103,2.0296171381
C,0,2.6091999666,0.4147709459,1.2772400578
H,0,1.3611218833,-0.1719476355,3.0202346761
H,0,3.1161437039,1.1695901319,1.8947736725
H,0,3.2997557114,-0.4436765451,1.2415019812
H,0,-0.5876337306,-0.7770235303,-0.6175305579
H,0,-0.5258733521,0.956293793,-0.3886578213
C,0,1.3922304197,0.0716256914,-0.9062641748

H,0,1.2657480322,0.4277861455,-1.9361173851
C,0,2.3803156671,0.9594585669,-0.1407254571
H,0,1.8008236548,-0.9466142618,-0.972203669
H,0,3.3338323736,1.0334172658,-0.6779847495
H,0,1.9725485613,1.9781062869,-0.0765317944
H,0,-1.9024602814,0.1888010362,1.8678624227
H,0,-1.5051850724,-1.5131457772,1.6605226874
H,0,-0.9491490411,-0.6483687631,3.1087054046

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.167965	E(Thermal)=	0.175216
E(QCISD(T))=	-273.071664	E(Empiric)=	-0.135200
DE(Plus)=	-0.013561	DE(2DF)=	-0.257520
E(Delta-G3)=	-0.387222	E(G3-Empiric)=	-0.135200
G3(0 K)=	-273.697202	G3 Energy=	-273.689951
G3 Enthalpy=	-273.689007	G3 Free Energy=	-273.727974

For Anharmonic Corrections of 4d-1

Zero-point vibrational energy 459366.8 (Joules/Mol)
109.79129 (Kcal/Mol)
Vibrational temperatures: 184.67 267.29 364.46 437.46 477.51
(Kelvin) 619.78 635.03 726.87 904.11 1109.86
1181.54 1209.88 1252.39 1304.96 1364.11
1413.68 1476.24 1528.88 1541.08 1598.62
1605.26 1696.47 1699.80 1745.41 1844.50
1884.23 1946.50 1994.98 2006.00 2016.15
2034.14 2074.91 2164.30 2171.63 2175.55
2186.04 2191.53 2204.00 2520.76 4314.87
4315.23 4349.17 4355.50 4360.69 4377.60
4383.82 4410.98 4426.57 4433.03 4485.73
4524.36

Zero-point correction=	0.174964 (Hartree/Particle)
Thermal correction to Energy=	0.181968
Thermal correction to Enthalpy=	0.182912
Thermal correction to Gibbs Free Energy=	0.144366
Sum of electronic and zero-point Energies=	-273.793031
Sum of electronic and thermal Energies=	-273.786026
Sum of electronic and thermal Enthalpies=	-273.785082
Sum of electronic and thermal Free Energies=	-273.823628

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	114.187	27.079	81.127

ZPE(harm) = 0.45937D+03 kJ/mol ZPE(anh)= 0.45261D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.49303D-79	0.91778D-78	
QZvib	0.14803D+02	0.18071D+02	
Energy	0.47776D+03	0.47139D+03	kJ/mol
Enthalpy	0.48024D+03	0.47386D+03	kJ/mol
Entropy	0.33944D+03	0.34238D+03	J/(mol K)
Sp.Heat(V)	0.11330D+03	0.11567D+03	J/(mol K)
Sp.Heat(P)	0.12161D+03	0.12398D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.49303D-79	0.91778D-78	
QZvib	0.14803D+02	0.18071D+02	
Energy	0.47776D+03	0.47139D+03	kJ/mol
Enthalpy	0.48024D+03	0.47386D+03	kJ/mol
Entropy	0.33944D+03	0.34238D+03	J/(mol K)
Sp.Heat(V)	0.11330D+03	0.11567D+03	J/(mol K)
Sp.Heat(P)	0.12161D+03	0.12398D+03	J/(mol K)

4d-2 Complex

B3LYP/6-31+G**

E(RB3LYP) = -300.622958261

Zero-point correction= 0.205794 (Hartree/Particle)
Thermal correction to Energy= 0.215114
Thermal correction to Enthalpy= 0.216058
Thermal correction to Gibbs Free Energy= 0.172636
Sum of electronic and ZPE= -300.417165
Sum of electronic and thermal Energies= -300.407844
Sum of electronic and thermal Enthalpies= -300.406900
Sum of electronic and thermal Free Energies= -300.450322

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.986	36.259	91.389

C,0,0.007726772,0.158450778,-0.1750505782
C,0,0.1005741938,-0.0491893197,1.3319174521

C,0,1.2938262258,0.113987055,1.9892603937
B,0,0.2506130249,1.8057348626,2.3597540449
C,0,-1.0815610649,-0.7165772209,1.9910712085
C,0,2.6058668635,0.4069936093,1.292765809
H,0,1.3714484297,-0.25290032,3.0094999432
H,0,0.1207316283,1.6397013727,3.5407674838
H,0,-0.7904904306,1.9699476428,1.7825417361
H,0,1.1204444542,2.531151478,1.9646148497
H,0,3.1906699157,1.116645095,1.8876654347
H,0,3.1791775121,-0.5333303758,1.2845321834
H,0,-0.6686373258,-0.6051650387,-0.5790855227
H,0,-0.4714049999,1.1230937257,-0.377157549
C,0,1.3715648838,0.0825113612,-0.8819909331
H,0,1.266345188,0.4206646922,-1.9191533313
C,0,2.427096712,0.9147085423,-0.1438832905
H,0,1.7014323819,-0.9650677587,-0.924783272
H,0,3.3868107798,0.8767312784,-0.6717958631
H,0,2.1142175729,1.965315841,-0.122518628
H,0,-2.0215606973,-0.2390614355,1.6982990893
H,0,-1.1246419651,-1.7639428135,1.6636014866
H,0,-1.0061500547,-0.6977240514,3.0806748527

B3LYP/6-31G*
E(RB3LYP) = -300.596059014

Zero-point correction= 0.207117 (Hartree/Particle)
Thermal correction to Energy= 0.216483
Thermal correction to Enthalpy= 0.217428
Thermal correction to Gibbs Free Energy= 0.173564
Sum of electronic and ZPE= -300.388942
Sum of electronic and thermal Energies= -300.379576
Sum of electronic and thermal Enthalpies= -300.378632
Sum of electronic and thermal Free Energies= -300.422495

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.845	36.024	92.318

C,0,0.0094546524,0.1391459551,-0.176124017
C,0,0.1054676688,-0.0566671047,1.3324427356
C,0,1.2978433272,0.1083197992,1.9867585697
B,0,0.2484899309,1.8120666033,2.3586251284
C,0,-1.0819729118,-0.7073543516,1.9984101751
C,0,2.6077473674,0.4027182281,1.2880914289

H,0,1.3761923872,-0.2449305134,3.0121548462
H,0,0.068166015,1.6240741898,3.530086216
H,0,-0.7599828843,2.006855795,1.7328856309
H,0,1.1557286725,2.5205696769,2.0166616645
H,0,3.1952729869,1.1085008096,1.885468992
H,0,3.1820343266,-0.5374685998,1.2699542819
H,0,-0.6542226519,-0.6386069076,-0.5763447308
H,0,-0.4874605426,1.0936973131,-0.3840436856
C,0,1.3731797716,0.0818890813,-0.8844113632
H,0,1.2632904321,0.4234471446,-1.9204348841
C,0,2.420114014,0.9209094488,-0.1429622668
H,0,1.7146828608,-0.9619814853,-0.9326284924
H,0,3.379052744,0.8999668309,-0.6741750056
H,0,2.0939000435,1.9675303092,-0.1098402123
H,0,-2.0165089934,-0.2102659526,1.7189601427
H,0,-1.1503434075,-1.7519594265,1.6642047468
H,0,-0.9960258093,-0.6977778435,3.087807099

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.198832	E(Thermal)=	0.208523
E(QCISD(T))=	-299.575204	E(Empiric)=	-0.155480
DE(Plus)=	-0.014414	DE(2DF)=	-0.300080
E(Delta-G3)=	-0.436191	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.282537	G3 Energy=	-300.272846
G3 Enthalpy=	-300.271902	G3 Free Energy=	-300.316363

For Anharmonic Corrections of 4d-2

Zero-point vibrational energy 543785.9 (Joules/Mol)
129.96794 (Kcal/Mol)
Vibrational temperatures: 67.56 205.94 288.00 298.46 326.61
(Kelvin) 392.46 452.46 488.79 499.20 615.25
647.90 756.58 906.77 1078.79 1138.07
1172.73 1195.32 1245.03 1276.41 1299.16
1403.95 1408.16 1483.45 1514.88 1540.76
1591.57 1606.64 1619.62 1686.87 1705.60
1715.75 1726.44 1748.10 1852.96 1895.79
1949.31 1997.17 2010.78 2020.51 2031.76
2072.78 2159.21 2167.77 2171.18 2184.42
2190.18 2205.82 2382.71 3647.33 3746.53
3792.52 4331.26 4361.55 4375.00 4389.36
4396.25 4431.58 4444.30 4449.58 4459.54
4473.51 4532.04 4578.69

Zero-point correction= 0.207117 (Hartree/Particle)
Thermal correction to Energy= 0.216483
Thermal correction to Enthalpy= 0.217428
Thermal correction to Gibbs Free Energy= 0.173567
Sum of electronic and zero-point Energies= -300.388942
Sum of electronic and thermal Energies= -300.379576
Sum of electronic and thermal Enthalpies= -300.378631
Sum of electronic and thermal Free Energies= -300.422492

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	135.845	36.024	92.313

ZPE(harm) = 0.54379D+03 kJ/mol ZPE(anh)= 0.53811D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.99787D-93	0.55461D-92	
QZvib	0.18456D+03	0.10386D+03	
Energy	0.56838D+03	0.56167D+03	kJ/mol
Enthalpy	0.57086D+03	0.56415D+03	kJ/mol
Entropy	0.38624D+03	0.37801D+03	J/(mol K)
Sp.Heat(V)	0.15072D+03	0.14967D+03	J/(mol K)
Sp.Heat(P)	0.15904D+03	0.15799D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.99787D-93	0.55461D-92	
QZvib	0.18456D+03	0.10386D+03	
Energy	0.56838D+03	0.56167D+03	kJ/mol
Enthalpy	0.57086D+03	0.56415D+03	kJ/mol
Entropy	0.38624D+03	0.37801D+03	J/(mol K)
Sp.Heat(V)	0.15072D+03	0.14967D+03	J/(mol K)
Sp.Heat(P)	0.15904D+03	0.15799D+03	J/(mol K)

4d-3 Complex
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.622945211

Zero-point correction= 0.205637 (Hartree/Particle)
Thermal correction to Energy= 0.215061
Thermal correction to Enthalpy= 0.216005

Thermal correction to Gibbs Free Energy= 0.171997
Sum of electronic and ZPE= -300.417308
Sum of electronic and thermal Energies= -300.407885
Sum of electronic and thermal Enthalpies= -300.406940
Sum of electronic and thermal Free Energies= -300.450948

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.953	36.335	92.621

C,0,-0.0544783382,0.1278674907,-0.0656070983
C,0,0.1685767133,-0.1765636466,1.4004142653
C,0,1.3742820392,-0.0239330174,2.0357419064
B,0,0.8571247385,-2.0689232186,1.6807595505
H,0,-0.7276190944,-0.2551119339,2.0105984741
C,0,2.6191573629,0.3849613027,1.2575928339
C,0,1.4776178431,0.0348143068,3.5400218712
H,0,0.5999185807,-0.3951589412,4.0275285525
H,0,1.9937713532,-2.2067300752,2.0443047243
H,0,0.6945466605,-2.3674504717,0.5303386802
H,0,3.1872041141,1.0893847415,1.8781302503
H,0,3.2654840369,-0.4904160732,1.1273973861
H,0,-0.7349682685,-0.6133260395,-0.4979816063
H,0,-0.5798841685,1.0945111201,-0.1157782437
C,0,1.2499674611,0.207026513,-0.8688056986
H,0,1.0541323731,0.652817138,-1.8506692312
C,0,2.3019836745,1.021412447,-0.1062094147
H,0,1.6298454186,-0.8061550383,-1.0463964254
H,0,3.2236805315,1.111038451,-0.6923173483
H,0,1.92652703,2.0428891884,0.0474048851
H,0,2.3679100989,-0.4917665686,3.8973348548
H,0,1.5674346644,1.0851425451,3.847641277
H,0,0.042154175,-2.4113192203,2.4913345545

B3LYP/6-31G*
E(RB+HF-LYP) = -300.596058961

Zero-point correction= 0.207116 (Hartree/Particle)
Thermal correction to Energy= 0.216483
Thermal correction to Enthalpy= 0.217427
Thermal correction to Gibbs Free Energy= 0.173563
Sum of electronic and ZPE= -300.388943
Sum of electronic and thermal Energies= -300.379576
Sum of electronic and thermal Enthalpies= -300.378632

Sum of electronic and thermal Free Energies= -300.422496

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.845	36.024	92.320

C,0,-0.0555605498,0.1302043656,-0.064439185
C,0,0.1676577032,-0.1726558003,1.4015433817
C,0,1.3726672971,-0.022051281,2.0358731586
B,0,0.8619951346,-2.0658035865,1.6774314841
H,0,-0.7291694181,-0.252925548,2.0111482879
C,0,2.6179143654,0.3884263787,1.25858754
C,0,1.476472511,0.0316186315,3.5402834686
H,0,0.5957372995,-0.3951392342,4.0265383253
H,0,2.0006305554,-2.206940712,2.0381261533
H,0,0.6957020171,-2.3620955044,0.5256671372
H,0,3.1840896435,1.0972147027,1.8771457326
H,0,3.267579242,-0.4852950608,1.1326061504
H,0,-0.7386896762,-0.6099596511,-0.4953265711
H,0,-0.5780770305,1.0988209148,-0.1177831109
C,0,1.2494216571,0.2025463443,-0.8665742196
H,0,1.055644222,0.6424502961,-1.8520297911
C,0,2.3011442649,1.01949372,-0.107468708
H,0,1.6273620776,-0.8129173938,-1.0366517704
H,0,3.2233767424,1.107411289,-0.6938465498
H,0,1.9257283822,2.0418763856,0.0422318073
H,0,2.3633980258,-0.5018892641,3.8970475021
H,0,1.572973742,1.0803344319,3.8540482605
H,0,0.0463707916,-2.407713424,2.4886205161

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.198832	E(Thermal)=	0.208523
E(QCISD(T))=	-299.575204	E(Empiric)=	-0.155480
DE(Plus)=	-0.014414	DE(2DF)=	-0.300080
E(Delta-G3)=	-0.436192	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.282537	G3 Energy=	-300.272846
G3 Enthalpy=	-300.271902	G3 Free Energy=	-300.316364

For Anharmonic Corrections of 4d-3

Zero-point vibrational energy 543785.2 (Joules/Mol)
129.96778 (Kcal/Mol)
Vibrational temperatures: 67.52 205.83 288.01 298.43 326.60
(Kelvin) 392.49 452.42 488.81 499.23 615.26
647.91 756.56 906.75 1078.80 1138.06

1172.70 1195.32 1245.04 1276.40 1299.17
1403.94 1408.16 1483.45 1514.91 1540.76
1591.56 1606.64 1619.61 1686.86 1705.59
1715.74 1726.47 1748.10 1852.95 1895.79
1949.31 1997.18 2010.78 2020.51 2031.77
2072.80 2159.20 2167.78 2171.18 2184.42
2190.17 2205.81 2382.72 3647.31 3746.53
3792.50 4331.25 4361.55 4375.01 4389.34
4396.24 4431.57 4444.32 4449.57 4459.53
4473.51 4532.06 4578.70

Zero-point correction= 0.207117 (Hartree/Particle)
Thermal correction to Energy= 0.216483
Thermal correction to Enthalpy= 0.217428
Thermal correction to Gibbs Free Energy= 0.173566
Sum of electronic and zero-point Energies= -300.388942
Sum of electronic and thermal Energies= -300.379576
Sum of electronic and thermal Enthalpies= -300.378631
Sum of electronic and thermal Free Energies= -300.422493

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	135.845	36.024	92.315

ZPE(harm) = 0.54379D+03 kJ/mol ZPE(anh)= 0.53815D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.99905D-93	0.53290D-92	
QZvib	0.18472D+03	0.10133D+03	
Energy	0.56838D+03	0.56169D+03	kJ/mol
Enthalpy	0.57086D+03	0.56417D+03	kJ/mol
Entropy	0.38625D+03	0.37775D+03	J/(mol K)
Sp.Heat(V)	0.15072D+03	0.14960D+03	J/(mol K)
Sp.Heat(P)	0.15904D+03	0.15792D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.99905D-93	0.53290D-92	
QZvib	0.18472D+03	0.10133D+03	
Energy	0.56838D+03	0.56169D+03	kJ/mol
Enthalpy	0.57086D+03	0.56417D+03	kJ/mol
Entropy	0.38625D+03	0.37775D+03	J/(mol K)
Sp.Heat(V)	0.15072D+03	0.14960D+03	J/(mol K)

Sp.Heat(P) 0.15904D+03 0.15792D+03 J/(mol K)

4d-4 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.618641910

Zero-point correction= 0.205961 (Hartree/Particle)
Thermal correction to Energy= 0.214068
Thermal correction to Enthalpy= 0.215012
Thermal correction to Gibbs Free Energy= 0.174306
Sum of electronic and ZPE= -300.412680
Sum of electronic and thermal Energies= -300.404574
Sum of electronic and thermal Enthalpies= -300.403629
Sum of electronic and thermal Free Energies= -300.444336

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.330	33.332	85.674

C,0,0.5364800865,1.4860448413,-0.4259915152
C,0,0.0306856798,0.0588451153,-0.1806174816
C,0,0.1307599695,-0.332952233,1.3053205601
C,0,1.4183070904,0.153028121,1.9853420651
C,0,2.3400131981,1.0298776828,1.3399931337
C,0,2.0176311293,1.5885698914,-0.0418298236
C,0,3.8178600482,0.9207731441,1.6616177233
B,0,1.3460855964,1.6836857041,2.7800257723
H,0,1.8620262737,-0.5594871254,2.6767788289
H,0,0.2597373863,2.1519251024,2.6016422512
H,0,2.1085121102,2.4506775796,2.167321596
H,0,0.0869120748,-1.425366985,1.3932340607
H,0,-0.7406969784,0.0519453939,1.8455018954
H,0,2.3859885946,2.6169284375,-0.1298258132
H,0,2.609698835,0.9865159578,-0.7478854595
H,0,0.4189958107,1.760678155,-1.4807608767
H,0,-0.0528775373,2.2022025531,0.1583754431
H,0,-1.0047236452,-0.0491199146,-0.5235953646
H,0,0.6342872491,-0.6334316182,-0.7853015258
H,0,1.8435970603,1.5962445217,3.8667326487
H,0,3.9773435535,0.6607923512,2.7107723396
H,0,4.2538681433,0.128244429,1.041241406

H,0,4.3491852712,1.8540108951,1.4479231361

B3LYP/6-31G*
E(RB+HF-LYP) = -300.590780673

Zero-point correction= 0.207416 (Hartree/Particle)
Thermal correction to Energy= 0.215460
Thermal correction to Enthalpy= 0.216404
Thermal correction to Gibbs Free Energy= 0.175788
Sum of electronic and ZPE= -300.383365
Sum of electronic and thermal Energies= -300.375321
Sum of electronic and thermal Enthalpies= -300.374377
Sum of electronic and thermal Free Energies= -300.414992

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.203	32.957	85.483

C,0,0.535747678,1.4878023276,-0.4224796022
C,0,0.0331397673,0.0597186179,-0.1796088028
C,0,0.1325697822,-0.3337678258,1.3055832236
C,0,1.4158936276,0.1574244354,1.9911569512
C,0,2.3385046938,1.0375343286,1.3433772889
C,0,2.017238861,1.5897718248,-0.0416369918
C,0,3.8167452927,0.9217005597,1.6621058966
B,0,1.3382563822,1.6749983907,2.7818969533
H,0,1.8666662693,-0.5622459578,2.6711886884
H,0,0.2592219988,2.1608296494,2.598278081
H,0,2.1079285993,2.437388276,2.1584638887
H,0,0.0905958909,-1.427012665,1.3908229429
H,0,-0.7422880768,0.0467782721,1.8439096785
H,0,2.3883813611,2.6170203291,-0.1370872072
H,0,2.6070956819,0.9828301448,-0.7460870558
H,0,0.4153954761,1.7658379427,-1.4765814212
H,0,-0.0526376848,2.2021140181,0.1657878878
H,0,-1.0019341832,-0.0505006803,-0.5244446331
H,0,0.6391972971,-0.6300189315,-0.7852952092
H,0,1.8444318816,1.6032001801,3.8665002914
H,0,3.9768513477,0.6658806802,2.7128415701
H,0,4.2477682631,0.1230810341,1.045032788
H,0,4.354906793,1.8502670493,1.4422897927

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199119	E(Thermal)=	0.207482

E(QCISD(T))=	-299.570741	E(Empiric)=	-0.155480
DE(Plus)=	-0.014624	DE(2DF)=	-0.301450
E(Delta-G3)=	-0.435343	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.278519	G3 Energy=	-300.270156
G3 Enthalpy=	-300.269212	G3 Free Energy=	-300.310366

For Anharmonic Corrections of 4d-4

Zero-point vibrational energy 544573.3 (Joules/Mol)
130.15614 (Kcal/Mol)
Vibrational temperatures: 173.90 276.29 344.64 427.36 459.66
(Kelvin) 480.03 564.61 639.02 697.27 780.60
815.58 909.36 1044.07 1151.72 1187.32
1201.14 1254.31 1307.23 1334.34 1411.64
1450.36 1476.67 1521.34 1542.20 1597.47
1621.92 1629.29 1657.46 1715.36 1726.16
1731.38 1742.97 1865.88 1893.47 1937.40
1993.79 2004.95 2017.22 2022.77 2071.74
2134.12 2167.42 2187.58 2191.46 2192.71
2200.95 2214.19 3352.66 3681.84 3822.36
4341.68 4350.30 4387.79 4388.41 4393.66
4425.06 4431.30 4446.18 4457.50 4478.73
4524.45 4543.81

Zero-point correction= 0.207417 (Hartree/Particle)
Thermal correction to Energy= 0.215461
Thermal correction to Enthalpy= 0.216405
Thermal correction to Gibbs Free Energy= 0.175790
Sum of electronic and zero-point Energies= -300.383364
Sum of electronic and thermal Energies= -300.375320
Sum of electronic and thermal Enthalpies= -300.374375
Sum of electronic and thermal Free Energies= -300.414991

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	135.204	32.957	85.483

ZPE(harm) = 0.54128D+03 kJ/mol ZPE(anh)= 0.53358D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.37320D-93	0.92659D-92	
QZvib	0.25112D+02	0.27957D+02	
Energy	0.56240D+03	0.55495D+03	kJ/mol
Enthalpy	0.56488D+03	0.55742D+03	kJ/mol

Entropy	0.36597D+03	0.36768D+03	J/(mol K)
Sp.Heat(V)	0.13789D+03	0.14041D+03	J/(mol K)
Sp.Heat(P)	0.14621D+03	0.14872D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.37320D-93	0.92659D-92	
QZvib	0.25112D+02	0.27957D+02	
Energy	0.56240D+03	0.55495D+03	kJ/mol
Enthalpy	0.56488D+03	0.55742D+03	kJ/mol
Entropy	0.36597D+03	0.36768D+03	J/(mol K)
Sp.Heat(V)	0.13789D+03	0.14041D+03	J/(mol K)
Sp.Heat(P)	0.14621D+03	0.14872D+03	J/(mol K)

4d-5 Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -300.618352091

Zero-point correction= 0.205926 (Hartree/Particle)
Thermal correction to Energy= 0.214026
Thermal correction to Enthalpy= 0.214970
Thermal correction to Gibbs Free Energy= 0.174216
Sum of electronic and ZPE= -300.412427
Sum of electronic and thermal Energies= -300.404326
Sum of electronic and thermal Enthalpies= -300.403382
Sum of electronic and thermal Free Energies= -300.444136

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.303	33.257	85.774

C,0,-0.005665854,0.3224123897,-0.1556932957
C,0,0.0538030655,0.1180260641,1.367759007
C,0,1.3070869487,0.2255622893,2.0459292993
B,0,0.4236887828,1.6542513801,2.371464142
C,0,-1.030231957,-0.7580313251,1.9646077238
C,0,2.6296156292,0.3640518735,1.2960220252
H,0,1.3839138708,-0.3515239377,2.9657634112
H,0,0.1270078539,1.6736497576,3.5327923315
H,0,-0.6741504703,1.541952979,1.801470244
H,0,0.937135691,2.5754653663,1.8012673274
H,0,3.3021260432,1.0305993215,1.847702924

H,0,3.1139769886,-0.624144808,1.2845819266
H,0,-0.7736692598,-0.3477706827,-0.5590820808
H,0,-0.3351246823,1.3414503205,-0.3824467265
C,0,1.3439886583,0.0664713018,-0.8469711704
H,0,1.2654421237,0.3486589209,-1.9034337827
C,0,2.4671161288,0.8442750682,-0.1523335612
H,0,1.5768590233,-1.0076014125,-0.8241019181
H,0,3.4138164013,0.716798636,-0.6901656083
H,0,2.2337417227,1.9163165408,-0.1699072176
H,0,-2.0286368321,-0.4532677757,1.6344232814
H,0,-0.8629317298,-1.7916351718,1.6363751487
H,0,-1.0002271467,-0.7364080958,3.0568745691

B3LYP/6-31G*
E(RB+HF-LYP) = -300.590456211

Zero-point correction= 0.207345 (Hartree/Particle)
Thermal correction to Energy= 0.215400
Thermal correction to Enthalpy= 0.216344
Thermal correction to Gibbs Free Energy= 0.175637
Sum of electronic and ZPE= -300.383111
Sum of electronic and thermal Energies= -300.375057
Sum of electronic and thermal Enthalpies= -300.374112
Sum of electronic and thermal Free Energies= -300.414819

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.165	32.910	85.675

C,0,-0.0068181567,0.3275667457,-0.1553935629
C,0,0.0511366622,0.1254283274,1.369181234
C,0,1.3067299246,0.2342101671,2.050275147
B,0,0.4330679281,1.6559696549,2.3728847607
C,0,-1.0271078195,-0.7599984942,1.9631681367
C,0,2.6284835848,0.3608761462,1.2969099862
H,0,1.3826746381,-0.3522735899,2.964865275
H,0,0.1232508959,1.6822252715,3.5313713904
H,0,-0.6688693963,1.5293282287,1.7992385203
H,0,0.9284957884,2.5824696152,1.7933907728
H,0,3.3086038926,1.0220764681,1.8466006933
H,0,3.1069260591,-0.6306961735,1.2822312351
H,0,-0.7773988757,-0.3396124061,-0.5604379838
H,0,-0.3320881292,1.3478007292,-0.3841097084

C,0,1.3423899496,0.066672112,-0.8444649915
H,0,1.2653190288,0.3462717987,-1.9022221347
C,0,2.4656458873,0.8433852645,-0.1499919216
H,0,1.5726429329,-1.0081853216,-0.8188246429
H,0,3.4122968739,0.7168396898,-0.6891503647
H,0,2.2320745327,1.915749385,-0.165754795
H,0,-2.0286051502,-0.4652095833,1.6314314769
H,0,-0.8507936654,-1.7928941414,1.6355887283
H,0,-0.9993763862,-0.738440894,3.0561107487

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199051	E(Thermal)=	0.207424
E(QCISD(T))=	-299.570270	E(Empiric)=	-0.155480
DE(Plus)=	-0.014804	DE(2DF)=	-0.301341
E(Delta-G3)=	-0.435099	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.277943	G3 Energy=	-300.269570
G3 Enthalpy=	-300.268626	G3 Free Energy=	-300.309871

For Anharmonic Corrections of 4d-5

Zero-point vibrational energy 544385.8 (Joules/Mol)
130.11134 (Kcal/Mol)
Vibrational temperatures: 156.23 259.03 370.54 417.83 467.59
(Kelvin) 488.26 540.89 638.23 665.11 814.19
874.09 921.10 1053.93 1124.70 1173.67
1211.86 1252.65 1310.15 1326.72 1401.17
1456.83 1482.43 1519.58 1542.04 1603.79
1618.14 1624.57 1674.18 1692.38 1723.65
1735.32 1740.46 1864.38 1905.40 1934.05
1992.13 1994.62 2009.86 2023.84 2072.25
2138.89 2176.79 2183.47 2188.13 2192.14
2197.06 2209.37 3356.91 3669.49 3814.16
4331.70 4359.44 4382.70 4385.66 4399.71
4426.53 4430.58 4444.31 4463.48 4475.52
4519.42 4525.70

Zero-point correction=	0.207346 (Hartree/Particle)
Thermal correction to Energy=	0.215400
Thermal correction to Enthalpy=	0.216344
Thermal correction to Gibbs Free Energy=	0.175637
Sum of electronic and zero-point Energies=	-300.383111
Sum of electronic and thermal Energies=	-300.375056
Sum of electronic and thermal Enthalpies=	-300.374112
Sum of electronic and thermal Free Energies=	-300.414819

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	135.166	32.910	85.675

ZPE(harm) = 0.54093D+03 kJ/mol ZPE(anh)= 0.53362D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.46877D-93	0.83065D-92	
QZvib	0.27351D+02	0.25486D+02	
Energy	0.56207D+03	0.55491D+03	kJ/mol
Enthalpy	0.56455D+03	0.55739D+03	kJ/mol
Entropy	0.36678D+03	0.36665D+03	J/(mol K)
Sp.Heat(V)	0.13769D+03	0.14001D+03	J/(mol K)
Sp.Heat(P)	0.14601D+03	0.14832D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.46877D-93	0.83065D-92	
QZvib	0.27351D+02	0.25486D+02	
Energy	0.56207D+03	0.55491D+03	kJ/mol
Enthalpy	0.56455D+03	0.55739D+03	kJ/mol
Entropy	0.36678D+03	0.36665D+03	J/(mol K)
Sp.Heat(V)	0.13769D+03	0.14001D+03	J/(mol K)
Sp.Heat(P)	0.14601D+03	0.14832D+03	J/(mol K)

4d-6 Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -300.614530179

Zero-point correction= 0.205941 (Hartree/Particle)
Thermal correction to Energy= 0.214083
Thermal correction to Enthalpy= 0.215027
Thermal correction to Gibbs Free Energy= 0.174241
Sum of electronic and ZPE= -300.408589
Sum of electronic and thermal Energies= -300.400447
Sum of electronic and thermal Enthalpies= -300.399503
Sum of electronic and thermal Free Energies= -300.440289

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	134.339	33.293	85.842

C,0,-0.0343445836,0.3000608944,-0.1747683042
C,0,0.0621590369,0.1128720968,1.3419040027
C,0,1.3038851867,0.1445215472,2.0498976226
B,0,0.441811905,1.5971885887,2.3644807178
H,0,-0.7424280838,-0.4643619336,1.7933155032
C,0,2.6089695744,0.3218220094,1.265749319
C,0,1.4553231807,-0.734041277,3.2871989077
H,0,0.1546156462,1.6183034136,3.5257358779
H,0,-0.6733545176,1.4970291204,1.8174680467
H,0,0.9595633027,2.5141708822,1.795327995
H,0,3.2966580784,0.9568984551,1.8365746916
H,0,3.0883197885,-0.6676156584,1.1995415493
H,0,-0.7745534374,-0.4128007489,-0.5563218158
H,0,-0.4200909612,1.2985031881,-0.4058789741
C,0,1.3165088591,0.101291939,-0.8825286668
H,0,1.2295792138,0.426613457,-1.9257060515
C,0,2.4286591856,0.8667551025,-0.1573096679
H,0,1.5692748819,-0.9680217492,-0.9055298704
H,0,3.3750788475,0.7788972977,-0.7035605056
H,0,2.1783487474,1.9341764924,-0.1244363786
H,0,2.1800690693,-0.3007621548,3.9848661016
H,0,0.5082564265,-0.8436180132,3.8232748015
H,0,1.814447653,-1.7354869494,3.0120330982

B3LYP/6-31G*
E(RB+HF-LYP) = -300.586970385

Zero-point correction= 0.207430 (Hartree/Particle)
Thermal correction to Energy= 0.215519
Thermal correction to Enthalpy= 0.216463
Thermal correction to Gibbs Free Energy= 0.175750
Sum of electronic and ZPE= -300.379540
Sum of electronic and thermal Energies= -300.371452
Sum of electronic and thermal Enthalpies= -300.370507
Sum of electronic and thermal Free Energies= -300.411220

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.240	32.942	85.687

C,0,-0.0344168828,0.3021769617,-0.1744520346
C,0,0.061481628,0.1156399254,1.3430939072
C,0,1.3051343924,0.150697852,2.0526933648

B,0,0.4490739107,1.5966248171,2.3662796237
H,0,-0.739661807,-0.4690560211,1.7921488508
C,0,2.6091854097,0.3214128176,1.2658654537
C,0,1.4550948227,-0.7329553281,3.2861524755
H,0,0.1494762643,1.6228498189,3.5253886709
H,0,-0.6691596693,1.4850243434,1.8154587508
H,0,0.9538148022,2.5186271905,1.7913897172
H,0,3.3021024152,0.9539728965,1.8339100473
H,0,3.0865934128,-0.6694094462,1.1976527003
H,0,-0.7768853347,-0.4081123824,-0.557621312
H,0,-0.4169328735,1.3020466661,-0.4059535656
C,0,1.3161948777,0.1003605734,-0.8806429935
H,0,1.2298046914,0.4230025409,-1.9251934313
C,0,2.4274617516,0.8667985697,-0.156308357
H,0,1.5681201714,-0.9694724705,-0.900920617
H,0,3.3738596365,0.7808698765,-0.7039043536
H,0,2.1754223747,1.934146298,-0.1225461246
H,0,2.178966148,-0.3030248591,3.987626715
H,0,0.5068874846,-0.8452724608,3.8210921118
H,0,1.8151393733,-1.7345521794,3.0101184

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199133	E(Thermal)=	0.207539
E(QCISD(T))=	-299.567132	E(Empiric)=	-0.155480
DE(Plus)=	-0.014395	DE(2DF)=	-0.301232
E(Delta-G3)=	-0.435233	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.274339	G3 Energy=	-300.265933
G3 Enthalpy=	-300.264989	G3 Free Energy=	-300.306240

For Anharmonic Corrections of 4d-6

Zero-point vibrational energy 544607.3 (Joules/Mol)
130.16427 (Kcal/Mol)
Warning -- explicit consideration of 11 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 183.14 251.21 335.50 415.15 455.64
(Kelvin) 491.05 542.20 635.11 687.12 731.88
879.13 899.81 1030.85 1155.88 1190.14
1213.51 1259.29 1309.71 1344.91 1423.82
1476.35 1506.03 1533.49 1550.66 1583.99
1603.04 1636.84 1662.00 1712.30 1721.76
1730.64 1814.76 1870.15 1897.81 1933.25
1993.32 2000.36 2007.06 2022.77 2082.40
2124.96 2173.07 2186.10 2186.58 2190.82
2205.38 2220.34 3328.91 3689.91 3834.66

4319.78 4357.23 4362.98 4389.42 4400.39
4420.05 4432.02 4447.05 4453.40 4461.42
4497.17 4546.63

Zero-point correction= 0.207430 (Hartree/Particle)
Thermal correction to Energy= 0.215519
Thermal correction to Enthalpy= 0.216463
Thermal correction to Gibbs Free Energy= 0.175750
Sum of electronic and zero-point Energies= -300.379540
Sum of electronic and thermal Energies= -300.371452
Sum of electronic and thermal Enthalpies= -300.370507
Sum of electronic and thermal Free Energies= -300.411220

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	135.240	32.942	85.688

ZPE(harm) = 0.54077D+03 kJ/mol ZPE(anh)= 0.53212D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.48755D-93	0.17648D-91	
QZvib	0.26737D+02	0.29455D+02	
Energy	0.56201D+03	0.55389D+03	kJ/mol
Enthalpy	0.56449D+03	0.55637D+03	kJ/mol
Entropy	0.36683D+03	0.36944D+03	J/(mol K)
Sp.Heat(V)	0.13783D+03	0.14201D+03	J/(mol K)
Sp.Heat(P)	0.14614D+03	0.15032D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.48755D-93	0.17648D-91	
QZvib	0.26737D+02	0.29455D+02	
Energy	0.56201D+03	0.55389D+03	kJ/mol
Enthalpy	0.56449D+03	0.55637D+03	kJ/mol
Entropy	0.36683D+03	0.36944D+03	J/(mol K)
Sp.Heat(V)	0.13783D+03	0.14201D+03	J/(mol K)
Sp.Heat(P)	0.14614D+03	0.15032D+03	J/(mol K)

4d-7 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.613904712

Zero-point correction= 0.205944 (Hartree/Particle)
Thermal correction to Energy= 0.214092
Thermal correction to Enthalpy= 0.215037
Thermal correction to Gibbs Free Energy= 0.174225
Sum of electronic and ZPE= -300.407960
Sum of electronic and thermal Energies= -300.399812
Sum of electronic and thermal Enthalpies= -300.398868
Sum of electronic and thermal Free Energies= -300.439680

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.345	33.339	85.896

C,0,1.3617810022,0.2286749473,-0.8180929206
C,0,2.3534483341,1.1075568843,-0.0461146569
C,0,2.6756331108,0.5318433161,1.3454642951
C,0,1.4475807072,-0.0051759871,2.1112283049
C,0,0.2138173492,-0.1877777501,1.4179002857
C,0,0.0350707923,0.145091984,-0.0530880306
C,0,1.4016788584,0.4038517686,3.5800628065
B,0,1.149848703,-1.6980217556,1.8907860135
H,0,-0.6975348165,-0.1288917659,2.0111605605
H,0,0.5198223942,-0.0008123529,4.0851488099
H,0,1.9481342247,-2.1438139122,1.1221001732
H,0,0.0565785699,-1.8151527279,1.3043175394
H,0,3.1346610347,1.3205500058,1.9544495593
H,0,3.429678693,-0.256407892,1.2522655298
H,0,-0.6579329748,-0.5588416454,-0.5271647044
H,0,-0.455025378,1.130047305,-0.0774711954
H,0,1.1779539694,0.6408125022,-1.8170247249
H,0,1.7775123735,-0.7760216479,-0.9586278919
H,0,3.2815817695,1.2339452611,-0.6156144733
H,0,1.9167126808,2.1107907822,0.0649950071
H,0,2.284706437,0.0375290851,4.1145379014
H,0,1.3839842214,1.4982591825,3.677243492
H,0,0.9343149439,-2.1929615872,2.9583833199

B3LYP/6-31G*
E(RB+HF-LYP) = -300.586462104

Zero-point correction= 0.207421 (Hartree/Particle)

Thermal correction to Energy= 0.215514
Thermal correction to Enthalpy= 0.216459
Thermal correction to Gibbs Free Energy= 0.175722
Sum of electronic and ZPE= -300.379041
Sum of electronic and thermal Energies= -300.370948
Sum of electronic and thermal Enthalpies= -300.370003
Sum of electronic and thermal Free Energies= -300.410740

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.237	32.990	85.737

C,0,1.3610294197,0.2250711994,-0.8159844178
C,0,2.3522243618,1.1053790859,-0.0461041567
C,0,2.6755183396,0.5324453777,1.346031286
C,0,1.450221179,-0.0110951779,2.1120854555
C,0,0.2135609805,-0.1926381351,1.4179248379
C,0,0.0341878565,0.1473741647,-0.0517645431
C,0,1.4004724948,0.4031957243,3.5789942824
B,0,1.1599102385,-1.6945511534,1.8921180578
H,0,-0.6976934177,-0.1302027206,2.01191315
H,0,0.5168011433,0.0001995957,4.0837241181
H,0,1.9494696652,-2.1457673349,1.1157031324
H,0,0.0615543746,-1.8030110567,1.3014416507
H,0,3.1323559225,1.324530921,1.9534418079
H,0,3.434066766,-0.2518378483,1.2532711039
H,0,-0.6641454263,-0.5503361097,-0.528329926
H,0,-0.4498961313,1.1357630505,-0.0726716263
H,0,1.1786502395,0.6332401041,-1.8173724122
H,0,1.7748072311,-0.7814465036,-0.9516602147
H,0,3.2801876196,1.2322795217,-0.6166606954
H,0,1.9143167814,2.1086299149,0.0631175707
H,0,2.281991006,0.038910199,4.1183682365
H,0,1.3824032626,1.498269711,3.6756686326
H,0,0.9320130932,-2.1993285296,2.9535896699

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199124	E(Thermal)=	0.207535
E(QCISD(T))=	-299.566184	E(Empiric)=	-0.155480
DE(Plus)=	-0.014421	DE(2DF)=	-0.301555
E(Delta-G3)=	-0.435079	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.273595	G3 Energy=	-300.265184
G3 Enthalpy=	-300.264240	G3 Free Energy=	-300.305515

For Anharmonic Correction of 4d-7

Zero-point vibrational energy 544607.3 (Joules/Mol)
130.16427 (Kcal/Mol)
Warning -- explicit consideration of 11 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 183.14 251.21 335.50 415.15 455.64
(Kelvin) 491.05 542.20 635.11 687.12 731.88
879.13 899.81 1030.85 1155.88 1190.14
1213.51 1259.29 1309.71 1344.91 1423.82
1476.35 1506.03 1533.49 1550.66 1583.99
1603.04 1636.84 1662.00 1712.30 1721.76
1730.64 1814.76 1870.15 1897.81 1933.25
1993.32 2000.36 2007.06 2022.77 2082.40
2124.96 2173.07 2186.10 2186.58 2190.82
2205.38 2220.34 3328.91 3689.91 3834.66
4319.78 4357.23 4362.98 4389.42 4400.39
4420.05 4432.02 4447.05 4453.40 4461.42
4497.17 4546.63

Zero-point correction= 0.207430 (Hartree/Particle)
Thermal correction to Energy= 0.215519
Thermal correction to Enthalpy= 0.216463
Thermal correction to Gibbs Free Energy= 0.175750
Sum of electronic and zero-point Energies= -300.379540
Sum of electronic and thermal Energies= -300.371452
Sum of electronic and thermal Enthalpies= -300.370507
Sum of electronic and thermal Free Energies= -300.411220

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	135.240	32.942	85.688

ZPE(harm) = 0.54077D+03 kJ/mol ZPE(anh)= 0.53212D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.48755D-93	0.17648D-91	
QZvib	0.26737D+02	0.29455D+02	
Energy	0.56201D+03	0.55389D+03	kJ/mol
Enthalpy	0.56449D+03	0.55637D+03	kJ/mol
Entropy	0.36683D+03	0.36944D+03	J/(mol K)
Sp.Heat(V)	0.13783D+03	0.14201D+03	J/(mol K)
Sp.Heat(P)	0.14614D+03	0.15032D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.48755D-93	0.17648D-91	
QZvib	0.26737D+02	0.29455D+02	
Energy	0.56201D+03	0.55389D+03	kJ/mol
Enthalpy	0.56449D+03	0.55637D+03	kJ/mol
Entropy	0.36683D+03	0.36944D+03	J/(mol K)
Sp.Heat(V)	0.13783D+03	0.14201D+03	J/(mol K)
Sp.Heat(P)	0.14614D+03	0.15032D+03	J/(mol K)

4d-8 Variational Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -300.611201718

Zero-point correction= 0.201290 (Hartree/Particle)
Thermal correction to Energy= 0.211991
Thermal correction to Enthalpy= 0.212935
Thermal correction to Gibbs Free Energy= 0.164324
Sum of electronic and zero-point Energies= -300.409912
Sum of electronic and thermal Energies= -300.399211
Sum of electronic and thermal Enthalpies= -300.398266
Sum of electronic and thermal Free Energies= -300.446878

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	133.026	37.534	102.312

B3LYP/6-31G*

E(RB+HF-LYP) = -300.583308869

Zero-point correction= 0.202578 (Hartree/Particle)
Thermal correction to Energy= 0.213423
Thermal correction to Enthalpy= 0.214368
Thermal correction to Gibbs Free Energy= 0.164592
Sum of electronic and ZPE= -300.380731
Sum of electronic and thermal Energies= -300.369885
Sum of electronic and thermal Enthalpies= -300.368941
Sum of electronic and thermal Free Energies= -300.418717

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	133.925	37.375	104.762

C,0,-0.64613,0.74852,-1.13044
C,0,0.13283,0.94419,0.157
C,0,0.0201,0.08745,1.18486
B,0,3.34982,-1.06217,-0.21906
C,0,1.01578,2.16445,0.22004
C,0,-0.86323,-1.13718,1.18299
H,0,0.5766,0.28785,2.10067
H,0,3.71554,-1.15478,0.91358
H,0,3.54535,-0.05446,-0.82876
H,0,2.82021,-1.98944,-0.75328
H,0,-0.32971,-1.9813,1.64112
H,0,-1.73506,-0.95554,1.83257
H,0,-1.03915,1.71895,-1.46666
H,0,0.04817,0.42716,-1.92321
C,0,-1.79328,-0.26424,-0.99413
H,0,-2.17548,-0.53412,-1.98622
C,0,-1.33498,-1.51161,-0.22975
H,0,-2.62696,0.2034,-0.45155
H,0,-2.14211,-2.25246,-0.17637
H,0,-0.50599,-1.98424,-0.77495
H,0,1.73803,2.17807,-0.6078
H,0,0.42106,3.08451,0.12913
H,0,1.57697,2.2144,1.15884

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194475	E(Thermal)=	0.205610
E(QCISD(T))=	-299.559931	E(Empiric)=	-0.155480
DE(Plus)=	-0.015760	DE(2DF)=	-0.296030
E(Delta-G3)=	-0.435587	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.268313	G3 Energy=	-300.257178
G3 Enthalpy=	-300.256234	G3 Free Energy=	-300.306632

4d-9 Product
B3LYP/6-31+G**
E(RB3LYP) = -300.648136811

Zero-point correction= 0.207765 (Hartree/Particle)
Thermal correction to Energy= 0.216681

Thermal correction to Enthalpy= 0.217625
Thermal correction to Gibbs Free Energy= 0.175125
Sum of electronic and ZPE= -300.440372
Sum of electronic and thermal Energies= -300.431456
Sum of electronic and thermal Enthalpies= -300.430512
Sum of electronic and thermal Free Energies= -300.473012

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.969	34.980	89.449

C,0,2.035270498,0.5059343637,1.0337007343
C,0,3.0209376321,-0.0074747656,2.0998743869
C,0,2.2760540884,-0.6252040378,3.305548474
C,0,1.220975104,0.3773849914,3.8887750476
C,0,0.2538390462,0.8751501105,2.8002550036
C,0,1.0056739242,1.4880511974,1.6118121728
B,0,3.1533981731,-0.9909395924,4.5459939809
H,0,1.7356509399,1.2459389494,4.3259675409
C,0,4.0201956149,-1.0039059424,1.4958528321
H,0,1.5077716057,-0.3550579941,0.5946834886
H,0,0.6541689331,-0.0945526698,4.7006103604
H,0,-0.3546905376,0.0294286451,2.4501089262
H,0,-0.4400677058,1.6075497936,3.2321697403
H,0,1.5207901255,2.402090751,1.9418857252
H,0,0.2959242745,1.7950363065,0.8335133944
H,0,2.5901613187,0.979724639,0.2130952098
H,0,3.591451055,0.8579412385,2.4737835822
H,0,2.7784011457,-1.8023051043,5.3434617659
H,0,4.1699623839,-0.3980737217,4.7774253402
H,0,1.7063144168,-1.5020289468,2.9562247599
H,0,4.7621731886,-1.3257817615,2.2368397515
H,0,3.5047746083,-1.9005367663,1.1280951934
H,0,4.5641301668,-0.5640406833,0.6518105888

B3LYP/6-31G*
E(RB3LYP) = -300.621232421

Zero-point correction= 0.209283 (Hartree/Particle)
Thermal correction to Energy= 0.218151
Thermal correction to Enthalpy= 0.219095
Thermal correction to Gibbs Free Energy= 0.176679
Sum of electronic and ZPE= -300.411950
Sum of electronic and thermal Energies= -300.403081

Sum of electronic and thermal Enthalpies= -300.402137
Sum of electronic and thermal Free Energies= -300.444554

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.892	34.684	89.273

C,0,2.0343579927,0.5043804126,1.0333378202
C,0,3.0202216931,-0.0075462951,2.0995707621
C,0,2.2742070031,-0.6263888982,3.3040194802
C,0,1.2235136691,0.3797023622,3.8883397618
C,0,0.2553368316,0.8749934218,2.8006708319
C,0,1.0065257247,1.4872931872,1.6121186538
B,0,3.1518495963,-0.9922392245,4.5443689026
H,0,1.7417978127,1.2481638194,4.321891349
C,0,4.0195676751,-1.0036280387,1.497144132
H,0,1.5057273388,-0.3566973278,0.5952802663
H,0,0.6580580203,-0.0882264386,4.704155703
H,0,-0.3528984592,0.0282527988,2.4515108684
H,0,-0.4399301937,1.6071604902,3.2319542903
H,0,1.5230363583,2.4007697545,1.9425571195
H,0,0.2963039313,1.7960627471,0.8343211849
H,0,2.5883832163,0.9771601016,0.2109490784
H,0,3.5897673939,0.8583575424,2.4741381556
H,0,2.7896551688,-1.8207191109,5.331405626
H,0,4.1557242038,-0.3817275801,4.7893588636
H,0,1.7009874483,-1.4999786553,2.9524243129
H,0,4.7604077802,-1.3257472247,2.2402315752
H,0,3.505531851,-1.9011422555,1.1283664572
H,0,4.5651279433,-0.5639265884,0.6533728053

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200911	E(Thermal)=	0.210098
E(QCISD(T))=	-299.601361	E(Empiric)=	-0.155480
DE(Plus)=	-0.013830	DE(2DF)=	-0.299941
E(Delta-G3)=	-0.435386	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.305086	G3 Energy=	-300.295899
G3 Enthalpy=	-300.294955	G3 Free Energy=	-300.337943

4d-10 Product
B3LYP/6-31+G**
E(RB3LYP) = -300.645816610

Zero-point correction= 0.207535 (Hartree/Particle)
Thermal correction to Energy= 0.216398
Thermal correction to Enthalpy= 0.217342
Thermal correction to Gibbs Free Energy= 0.175216
Sum of electronic and ZPE= -300.438282
Sum of electronic and thermal Energies= -300.429419
Sum of electronic and thermal Enthalpies= -300.428475
Sum of electronic and thermal Free Energies= -300.470600

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.792	35.251	88.661

C,0,2.041085461,0.5509049898,1.1042692902
C,0,2.8297035494,-0.0551444397,2.2776438946
C,0,1.8939016618,-0.6315674421,3.3643716871
C,0,0.9270955706,0.4731171996,3.8480628356
C,0,0.1252649442,1.0828316197,2.6855967141
C,0,1.0511951018,1.6234792352,1.5848522178
C,0,2.7452499568,-1.1466257796,4.5690936056
H,0,1.5063026841,1.2720398378,4.3384717832
H,0,3.5075714072,-0.8371807492,1.9126799612
H,0,1.4884663567,-0.2486110022,0.5872474588
H,0,0.2443791452,0.0688630529,4.6061935594
H,0,-0.5366816046,0.313677322,2.2588016756
H,0,-0.5297594553,1.8810485189,3.056341586
H,0,1.6158268986,2.4806102836,1.9806144598
H,0,0.4601283852,2.0017751185,0.7414980724
H,0,2.7312475154,0.9756251412,0.3647105978
H,0,3.4628537689,0.7287936973,2.7235377061
B,0,1.1819183207,-1.9658804101,2.950715584
H,0,0.154508829,-2.2972826328,3.4709459234
H,0,1.7065779569,-2.7281338857,2.1893166818
H,0,2.1235152637,-1.5472673002,5.3785020707
H,0,3.4640313159,-1.9195034476,4.2720612633
H,0,3.3201459668,-0.3077339271,4.9833713713

B3LYP/6-31G*
E(RB3LYP) = -300.618957163

Zero-point correction= 0.209029 (Hartree/Particle)
Thermal correction to Energy= 0.217856
Thermal correction to Enthalpy= 0.218800

Thermal correction to Gibbs Free Energy= 0.176725
Sum of electronic and ZPE= -300.409928
Sum of electronic and thermal Energies= -300.401101
Sum of electronic and thermal Enthalpies= -300.400157
Sum of electronic and thermal Free Energies= -300.442232

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.707	34.965	88.555

C,0,2.0443294464,0.5541837183,1.1076016675
C,0,2.8307509298,-0.0543144779,2.2804385131
C,0,1.8921092466,-0.6333680482,3.3628709041
C,0,0.9257286086,0.470665921,3.8478585201
C,0,0.1269247825,1.0826891583,2.6852805724
C,0,1.0557294317,1.6264397339,1.5894203425
C,0,2.7416381028,-1.148525707,4.5680556109
H,0,1.5035943829,1.2685354741,4.3421881732
H,0,3.5095530194,-0.8353956112,1.91386238
H,0,1.4908778104,-0.2444619796,0.5892866894
H,0,0.2403147129,0.0655604209,4.6037335595
H,0,-0.5329011781,0.313428882,2.254391403
H,0,-0.5304920593,1.8795874443,3.0560205811
H,0,1.6211519672,2.4810374039,1.9903215279
H,0,0.4673429294,2.0098534285,0.7459194484
H,0,2.7355351599,0.9792909118,0.3685432894
H,0,3.4642197198,0.7282620012,2.7289600258
B,0,1.1793155918,-1.9651431462,2.9427537547
H,0,0.1496581274,-2.2987171669,3.4595993591
H,0,1.703708657,-2.7268379984,2.1789748988
H,0,2.1183707547,-1.551922898,5.3756461365
H,0,3.4605755548,-1.9221662558,4.271361001
H,0,3.3164933016,-0.310846209,4.9858116419

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200668	E(Thermal)=	0.209821
E(QCISD(T))=	-299.600347	E(Empiric)=	-0.155480
DE(Plus)=	-0.014009	DE(2DF)=	-0.300451
E(Delta-G3)=	-0.435322	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.304942	G3 Energy=	-300.295789
G3 Enthalpy=	-300.294845	G3 Free Energy=	-300.337497

4d-11 Product
B3LYP/6-31+G**
E(RB3LYP) = -300.646391410

Zero-point correction= 0.207430 (Hartree/Particle)
Thermal correction to Energy= 0.216208
Thermal correction to Enthalpy= 0.217153
Thermal correction to Gibbs Free Energy= 0.174980
Sum of electronic and ZPE= -300.438961
Sum of electronic and thermal Energies= -300.430183
Sum of electronic and thermal Enthalpies= -300.429239
Sum of electronic and thermal Free Energies= -300.471412

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.673	34.885	88.760

C,0,2.0473646546,0.5240146089,1.0268346529
C,0,3.0155380915,0.0240563444,2.1176940204
C,0,2.2014904207,-0.6249945422,3.2691359042
C,0,1.21417261,0.4047075257,3.8662270138
C,0,0.2448550284,0.9122881557,2.7858750706
C,0,1.0002179828,1.5019470258,1.5844702028
H,0,2.9239250039,-0.9047700584,4.0747660756
H,0,1.7692067321,1.2610318454,4.2773640078
C,0,4.114094856,-0.8752481271,1.5388488624
H,0,1.539854744,-0.345276665,0.5793638126
H,0,0.6548813204,-0.0409491839,4.697101279
H,0,-0.3837950155,0.0743381265,2.4470086346
H,0,-0.4374401832,1.6611276951,3.2070759137
H,0,1.5085205188,2.4245503723,1.9009339729
H,0,0.2944870883,1.7913832241,0.795813444
H,0,2.6128317733,1.0027664773,0.216541414
H,0,3.5119873538,0.9141424439,2.537829295
B,0,1.6066422384,-2.0535714474,3.0616929136
H,0,0.7300604714,-2.43230436,3.7864414091
H,0,2.0529305467,-2.8357568592,2.2746000336
H,0,4.7833255589,-1.2451253079,2.3252411938
H,0,3.6974614908,-1.7452151267,1.0213575484
H,0,4.7245267138,-0.3194951675,0.8177263253

B3LYP/6-31G*
E(RB3LYP) = -300.619245701

Zero-point correction= 0.208885 (Hartree/Particle)
Thermal correction to Energy= 0.217645
Thermal correction to Enthalpy= 0.218589
Thermal correction to Gibbs Free Energy= 0.176407
Sum of electronic and ZPE= -300.410361
Sum of electronic and thermal Energies= -300.401601
Sum of electronic and thermal Enthalpies= -300.400657
Sum of electronic and thermal Free Energies= -300.442839

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.574	34.605	88.779

C,0,2.0475652372,0.5210143141,1.0278665478
C,0,3.0167898303,0.0255311998,2.1191196484
C,0,2.2054929064,-0.6240467607,3.2716702081
C,0,1.2165329781,0.4050158257,3.8670021364
C,0,0.2466490114,0.9088352817,2.7864227065
C,0,1.0011252225,1.4989258023,1.5854092496
H,0,2.9281655541,-0.8984721219,4.0780250738
H,0,1.770598213,1.262858574,4.2771328359
C,0,4.1154978102,-0.8737643935,1.542130461
H,0,1.5394619201,-0.3496802263,0.5829428219
H,0,0.657592129,-0.0399569695,4.6990931074
H,0,-0.3795908188,0.0683855211,2.4477011367
H,0,-0.4385599304,1.6561804318,3.2066795026
H,0,1.509774162,2.4214967549,1.9024725311
H,0,0.2949311656,1.7894388371,0.7969193675
H,0,2.611241286,0.9981628902,0.2147913341
H,0,3.5120053456,0.9175834858,2.5373680212
B,0,1.6007334017,-2.0488662159,3.0546144644
H,0,0.7286422061,-2.4314435343,3.7843634313
H,0,2.0323269703,-2.8264672733,2.2530588037
H,0,4.7900951021,-1.2351350456,2.3286466524
H,0,3.6991841827,-1.7498203712,1.0337222345
H,0,4.7208861148,-0.3221290063,0.8127907236

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200529	E(Thermal)=	0.209611
E(QCISD(T))=	-299.599527	E(Empiric)=	-0.155480
DE(Plus)=	-0.013676	DE(2DF)=	-0.300200
E(Delta-G3)=	-0.435859	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.304212	G3 Energy=	-300.295131
G3 Enthalpy=	-300.294186	G3 Free Energy=	-300.336938

4d-12 Product
B3LYP/6-31+G**
E(RB3LYP) = -300.645429448

Zero-point correction= 0.207248 (Hartree/Particle)
Thermal correction to Energy= 0.216097
Thermal correction to Enthalpy= 0.217042
Thermal correction to Gibbs Free Energy= 0.174780
Sum of electronic and ZPE= -300.438181
Sum of electronic and thermal Energies= -300.429332
Sum of electronic and thermal Enthalpies= -300.428388
Sum of electronic and thermal Free Energies= -300.470649

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.603	35.076	88.947

C,0,2.0569193011,0.4985484272,1.062739559
C,0,3.0534500086,0.0993628851,2.1743575359
C,0,2.3021867142,-0.4825654598,3.4044376413
C,0,1.1549486509,0.4327233873,3.8910034755
C,0,0.1900558456,0.8102153142,2.7557594605
C,0,0.9349866411,1.4251174066,1.5607690561
B,0,3.1772340084,-1.1592412699,4.4979834503
H,0,1.5776512342,1.3501116295,4.3237211697
H,0,3.6955620247,-0.6980925145,1.7757976313
H,0,1.6002065272,-0.4163952071,0.6578255296
H,0,0.610902415,-0.0619898275,4.7044882041
H,0,-0.3401936461,-0.0943443465,2.4212791812
H,0,-0.5771491049,1.5032071982,3.1238060719
H,0,1.3546071215,2.3971031366,1.8546086958
H,0,0.2335968314,1.6304138248,0.7424135988
H,0,2.5967036065,0.9702954771,0.2310230657
C,0,3.9820894221,1.2638668964,2.566001698
H,0,2.752353626,-1.3307442774,5.6052883017
H,0,4.250993535,-1.6159537215,4.2239946673
H,0,1.8150750504,-1.4283573829,3.0519928203
H,0,4.7278060269,0.938086615,3.3007305514
H,0,4.5229736297,1.6408153661,1.690184343

B3LYP/6-31G*
E(RB3LYP) = -300.618289927

Zero-point correction= 0.208725 (Hartree/Particle)

Thermal correction to Energy= 0.217545
Thermal correction to Enthalpy= 0.218489
Thermal correction to Gibbs Free Energy= 0.176260
Sum of electronic and ZPE= -300.409565
Sum of electronic and thermal Energies= -300.400745
Sum of electronic and thermal Enthalpies= -300.399801
Sum of electronic and thermal Free Energies= -300.442030

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.511	34.786	88.879

C,0,2.0564444738,0.4979370231,1.0621795181
C,0,3.0521424324,0.0969482434,2.1731503046
C,0,2.2986773511,-0.4883265673,3.400580834
C,0,1.1549472798,0.4301785287,3.8893772966
C,0,0.190562512,0.8083546415,2.7546916671
C,0,0.9364702278,1.4250372974,1.5619394465
B,0,3.1810795885,-1.1524839407,4.4987466677
H,0,1.5796846788,1.3473036343,4.3215110271
H,0,3.6957085213,-0.6993178119,1.7736406086
H,0,1.5983639301,-0.41629101,0.6561887176
H,0,0.6104428053,-0.0629201598,4.7042282183
H,0,-0.3390748271,-0.0962324271,2.4184369685
H,0,-0.5779525002,1.5004760622,3.1230962813
H,0,1.3582851674,2.3954768354,1.8590750114
H,0,0.2354998256,1.6344632897,0.743649782
H,0,2.5961772436,0.9701813747,0.2300877533
C,0,3.9785763579,1.2607436146,2.5682959906
H,0,2.7639571789,-1.3127013233,5.611700124
H,0,4.2563958798,-1.6087072542,4.2255679865
H,0,1.8074633112,-1.428619009,3.0422150808
H,0,4.7232398701,0.9341882799,3.3047750477
H,0,4.5211079956,1.6403106383,1.6939804668
H,0,3.4304006965,2.10342204,3.0041392008

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200376	E(Thermal)=	0.209518
E(QCISD(T))=	-299.598443	E(Empiric)=	-0.155480
DE(Plus)=	-0.013762	DE(2DF)=	-0.300345
E(Delta-G3)=	-0.435636	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.303290	G3 Energy=	-300.294148
G3 Enthalpy=	-300.293204	G3 Free Energy=	-300.336007

4d-13 Product
B3LYP/6-31+G**
E(RB3LYP) = -300.644746147

Zero-point correction= 0.207576 (Hartree/Particle)
Thermal correction to Energy= 0.216323
Thermal correction to Enthalpy= 0.217267
Thermal correction to Gibbs Free Energy= 0.175216
Sum of electronic and ZPE= -300.437170
Sum of electronic and thermal Energies= -300.428423
Sum of electronic and thermal Enthalpies= -300.427479
Sum of electronic and thermal Free Energies= -300.469530

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.745	34.841	88.503

C,0,2.0162621718,0.5589350027,1.0381613479
C,0,2.9947155149,0.0522210648,2.1236122879
C,0,2.1804258021,-0.5819433961,3.2848056626
C,0,1.1306425452,0.394612831,3.8643369779
C,0,0.173424696,0.8774384964,2.7620590006
C,0,0.9397231617,1.5100382069,1.5895470241
H,0,2.9003432287,-0.8341616018,4.1029048183
H,0,1.621364974,1.2667019566,4.3179634241
H,0,3.6028603664,-0.7427741459,1.6714614326
H,0,1.5182227745,-0.3115811573,0.5852036022
H,0,0.5663873584,-0.0973337294,4.6652685577
H,0,-0.4103721645,0.0197785876,2.3932571592
H,0,-0.5505830584,1.5923317249,3.1724702107
H,0,1.4075731523,2.4451029535,1.9266170641
H,0,0.2446363837,1.7878140298,0.7874021833
H,0,2.5762217705,1.0493326498,0.2313067483
C,0,3.9670802134,1.1507355105,2.5892692629
B,0,1.6876316948,-2.0427236329,3.055147194
H,0,0.7896886788,-2.4943691275,3.7079780446
H,0,2.2666486548,-2.7735339338,2.3018028055
H,0,4.6805312955,0.7551685888,3.3217844213
H,0,4.5433180989,1.5425280538,1.7426883732
H,0,3.4540456865,1.9980330678,3.055559397

B3LYP/6-31G*
E(RB3LYP) = -300.617639993

Zero-point correction= 0.209052 (Hartree/Particle)
Thermal correction to Energy= 0.217763
Thermal correction to Enthalpy= 0.218707
Thermal correction to Gibbs Free Energy= 0.176708
Sum of electronic and ZPE= -300.408588
Sum of electronic and thermal Energies= -300.399877
Sum of electronic and thermal Enthalpies= -300.398933
Sum of electronic and thermal Free Energies= -300.440932

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.648	34.546	88.394

C,0,2.0171322414,0.5540484,1.0401776693
C,0,2.9969142735,0.0522017831,2.1257471656
C,0,2.1848065069,-0.5814911602,3.288811282
C,0,1.1347022214,0.3954858522,3.8663240614
C,0,0.176721186,0.8746050596,2.7641551124
C,0,0.9414548826,1.5057047427,1.5906086452
H,0,2.9054303484,-0.8286609898,4.1067747509
H,0,1.6252230667,1.2690210078,4.3184042519
H,0,3.60774857,-0.742001657,1.6748815238
H,0,1.5184849131,-0.3187357575,0.5909870603
H,0,0.570741559,-0.0952279575,4.6688636751
H,0,-0.4055975311,0.014695,2.3969811076
H,0,-0.5491671903,1.5889408453,3.1734255085
H,0,1.4101011668,2.4412791436,1.9264010622
H,0,0.2454775343,1.7830263254,0.7884305177
H,0,2.5748895903,1.0423487253,0.2299393284
C,0,3.9650575047,1.1538991807,2.5895264897
B,0,1.6805118049,-2.0383868171,3.0471955233
H,0,0.7753213783,-2.4885684178,3.6928408393
H,0,2.2554317309,-2.7698154041,2.2898027963
H,0,4.6795627432,0.7623599939,3.3240115331
H,0,4.5409688754,1.5465043677,1.7423908482
H,0,3.4488756234,2.0011197336,3.0539262479

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200689	E(Thermal)=	0.209724
E(QCISD(T))=	-299.598100	E(Empiric)=	-0.155480
DE(Plus)=	-0.013573	DE(2DF)=	-0.300478
E(Delta-G3)=	-0.435901	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.302843	G3 Energy=	-300.293808
G3 Enthalpy=	-300.292863	G3 Free Energy=	-300.335435

4d-14 Product
B3LYP/6-31+G**
E(RB3LYP) = -300.642476935

Zero-point correction= 0.207391 (Hartree/Particle)
Thermal correction to Energy= 0.216417
Thermal correction to Enthalpy= 0.217361
Thermal correction to Gibbs Free Energy= 0.174784
Sum of electronic and ZPE= -300.435086
Sum of electronic and thermal Energies= -300.426060
Sum of electronic and thermal Enthalpies= -300.425115
Sum of electronic and thermal Free Energies= -300.467693

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.804	35.497	89.613

C,0,2.1204386713,0.5579767193,1.0711064525
C,0,3.1167982657,0.1601960514,2.1751381179
C,0,2.454084976,-0.4919698637,3.4182691092
C,0,1.2767278496,0.3911178423,3.912354648
C,0,0.2845621717,0.7882387009,2.8042999592
C,0,1.000776672,1.4549110075,1.620162519
B,0,3.4787470629,-0.8379145633,4.5503611194
H,0,1.6893538796,1.313736378,4.3471151622
H,0,3.8837911802,-0.5129822201,1.771109872
H,0,1.6771455038,-0.3409222251,0.6207527564
H,0,0.75074517,-0.1198384485,4.7290121875
H,0,-0.2579008543,-0.0982688083,2.4476676112
H,0,-0.4752134392,1.4634199381,3.2179310241
H,0,1.4342711336,2.4101905754,1.9524134887
H,0,0.2824855561,1.6976238235,0.8270891304
H,0,2.6558691423,1.0707407591,0.2620249227
H,0,3.6486111281,1.0677871004,2.4975303397
H,0,3.1210131595,-0.9263399917,5.6907600474
H,0,4.6161006818,-1.1062718044,4.2845295043
C,0,1.9536187042,-1.9372475862,3.0806254905
H,0,1.4852399323,-2.4181184859,3.9477984301
H,0,1.203502612,-1.9158968167,2.2829367563
H,0,2.7715288407,-2.5800760822,2.7335263513

B3LYP/6-31G*
E(RB3LYP) = -300.615580727

Zero-point correction= 0.208892 (Hartree/Particle)
Thermal correction to Energy= 0.217876
Thermal correction to Enthalpy= 0.218820
Thermal correction to Gibbs Free Energy= 0.176325
Sum of electronic and ZPE= -300.406688
Sum of electronic and thermal Energies= -300.397705
Sum of electronic and thermal Enthalpies= -300.396761
Sum of electronic and thermal Free Energies= -300.439256

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.719	35.208	89.439

C,0,2.1206651909,0.5560226835,1.0724053502
C,0,3.1175022775,0.1620695964,2.1766475682
C,0,2.4542592174,-0.4913969831,3.418424657
C,0,1.2783284048,0.3928199693,3.9129009485
C,0,0.2855355941,0.7861765712,2.8047964776
C,0,1.0011603158,1.4525885196,1.6208607127
B,0,3.4784732206,-0.8398540763,4.5503692922
H,0,1.6915047623,1.3170374144,4.3446040868
H,0,3.8875777441,-0.508398287,1.7727928718
H,0,1.6779489113,-0.3446814758,0.6242824242
H,0,0.7526762152,-0.1151247095,4.7322325293
H,0,-0.2549880177,-0.1022860891,2.4490598462
H,0,-0.4762751489,1.4605705178,3.2172298752
H,0,1.4348103257,2.4080233334,1.9532817276
H,0,0.2826510481,1.6956770415,0.8274657812
H,0,2.6549316248,1.0678861513,0.2613416525
H,0,3.6463988692,1.0717209438,2.499212423
H,0,3.1219603053,-0.9295764956,5.6921271846
H,0,4.6166585648,-1.1104481822,4.2857266064
C,0,1.9506104181,-1.9338076394,3.0769207746
H,0,1.4820986054,-2.4165707637,3.9436597655
H,0,1.19999981,-1.9102281802,2.2789532674
H,0,2.7678097413,-2.5781278603,2.7292191772

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200537	E(Thermal)=	0.209844
E(QCISD(T))=	-299.596717	E(Empiric)=	-0.155480
DE(Plus)=	-0.014129	DE(2DF)=	-0.300520
E(Delta-G3)=	-0.435237	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.301545	G3 Energy=	-300.292237
G3 Enthalpy=	-300.291293	G3 Free Energy=	-300.334370

See page 121 for structures of the 4e series

4e-1

B3LYP/6-31+G**
E(RB+HF-LYP) = -273.988536344

Zero-point correction= 0.173934 (Hartree/Particle)
Thermal correction to Energy= 0.180841
Thermal correction to Enthalpy= 0.181785
Thermal correction to Gibbs Free Energy= 0.143454
Sum of electronic and ZPE= -273.814602
Sum of electronic and thermal Energies= -273.807695
Sum of electronic and thermal Enthalpies= -273.806751
Sum of electronic and thermal Free Energies= -273.845083

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.480	27.121	80.676

C,0,-0.0604128551,0.2246720188,-0.1817934021
C,0,0.0170490262,0.0505151372,1.3437990285
C,0,1.4052095618,0.3233568278,1.8712753707
C,0,2.3668984496,0.9182712583,1.1523359994
C,0,2.1808452973,1.4268600989,-0.2621766402
C,0,0.6863488751,1.4886021802,-0.6287447586
H,0,2.6699795993,0.7100956685,-0.9434062546
H,0,3.3521677703,1.0613499028,1.5964768993
H,0,1.6194022822,0.0106753735,2.892496799
H,0,-0.2925868543,-0.9641244301,1.627997523
H,0,-0.6991345866,0.7255775599,1.8380254894
C,0,2.8727286666,2.7856736016,-0.4625387576
H,0,0.575844534,1.6412233228,-1.7096433163
H,0,0.2374672081,2.3652776378,-0.1389902049
H,0,-1.1070447613,0.2602193961,-0.5065629647
H,0,0.3913338995,-0.6507897062,-0.6683199416
H,0,2.7586202814,3.1347405513,-1.4953013841
H,0,2.4418398216,3.5445860208,0.2012304593
H,0,3.9454137844,2.7218875802,-0.2467599442

B3LYP/6-31G*
E(RB+HF-LYP) = -273.963001664

Zero-point correction= 0.175134 (Hartree/Particle)
Thermal correction to Energy= 0.182006
Thermal correction to Enthalpy= 0.182950

Thermal correction to Gibbs Free Energy= 0.144672
Sum of electronic and ZPE= -273.787868
Sum of electronic and thermal Energies= -273.780996
Sum of electronic and thermal Enthalpies= -273.780052
Sum of electronic and thermal Free Energies= -273.818330

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	114.210	26.871	80.563

C,0,-0.0590847741,0.2243729386,-0.1810985934
C,0,0.0177783626,0.0541923085,1.3444630067
C,0,1.4065569016,0.3254727054,1.8695141973
C,0,2.3672981747,0.9146463143,1.1500566591
C,0,2.1816341266,1.4243119647,-0.2637088373
C,0,0.6873142826,1.4871926446,-0.6298568311
H,0,2.6713068331,0.7103865312,-0.9482495805
H,0,3.3542394476,1.0578677825,1.5916612873
H,0,1.6191292722,0.0117253494,2.8913081563
H,0,-0.2954556975,-0.9596624249,1.6305178753
H,0,-0.6988717232,0.7312059703,1.8367861295
C,0,2.870394433,2.7848454026,-0.459658108
H,0,0.5758747233,1.6393993132,-1.7111958659
H,0,0.2385723219,2.3644866433,-0.1406798771
H,0,-1.1059436923,0.2581794652,-0.5070013941
H,0,0.3938098509,-0.6521522421,-0.6651031932
H,0,2.7557930021,3.137823743,-1.4915757663
H,0,2.437805505,3.5410905077,0.2066889318
H,0,3.9437976499,2.7232640824,-0.2434451964

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.168128	E(Thermal)=	0.175248
E(QCISD(T))=	-273.068297	E(Empiric)=	-0.135200
DE(Plus)=	-0.014301	DE(2DF)=	-0.257712
E(Delta-G3)=	-0.386760	E(G3-Empiric)=	-0.135200
G3(0 K)=	-273.694141	G3 Energy=	-273.687022
G3 Enthalpy=	-273.686077	G3 Free Energy=	-273.724773

CBS-QB3

C,0,-0.0593930384,0.2258511539,-0.181195888
C,0,0.0198111141,0.0548063554,1.3427525724
C,0,1.4070075663,0.3268383279,1.8673410855
C,0,2.3648114914,0.9154948402,1.1504099579

C,0,2.1803112218,1.4248123849,-0.2621951091
C,0,0.687923088,1.4863324751,-0.6308332568
H,0,2.6704356032,0.7108337029,-0.9420369647
H,0,3.3491910739,1.0571439266,1.5920468879
H,0,1.6200409163,0.0145989176,2.8868149564
H,0,-0.2892412944,-0.9574951743,1.6281897135
H,0,-0.6945015236,0.729020147,1.8363693931
C,0,2.8690490076,2.784057498,-0.4584928342
H,0,0.5787293252,1.6351977678,-1.7101571036
H,0,0.2402201365,2.3631376801,-0.1451091396
H,0,-1.1041355698,0.262091474,-0.5046432814
H,0,0.3900372308,-0.6494822793,-0.6651555432
H,0,2.7519630594,3.1371760006,-1.4873882384
H,0,2.4392657744,3.5374490575,0.2089517056
H,0,3.9404238175,2.7207847441,-0.2462459134

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.171831	E(Thermal)=	0.178797
E(SCF)=	-272.138497	DE(MP2)=	-1.165224
DE(CBS)=	-0.109775	DE(MP34)=	-0.076218
DE(CCSD)=	-0.036493	DE(Int)=	0.039169
DE(Empirical)=	-0.058643		
CBS-QB3 (0 K)=	-273.373850	CBS-QB3 Energy=	-273.366885
CBS-QB3 Enthalpy=	-273.365941	CBS-QB3 Free Energy=	-273.404369

4e-2
B3LYP/6-31+G**
E(RB+HF-LYP) = -273.987206373

Zero-point correction= 0.174044 (Hartree/Particle)
Thermal correction to Energy= 0.180949
Thermal correction to Enthalpy= 0.181894
Thermal correction to Gibbs Free Energy= 0.143581
Sum of electronic and ZPE= -273.813162
Sum of electronic and thermal Energies= -273.806257
Sum of electronic and thermal Enthalpies= -273.805313
Sum of electronic and thermal Free Energies= -273.843626

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.548	27.080	80.636

C,0,-0.0421380347,0.1179037714,-0.2380910715
C,0,0.0938395087,-0.0597298178,1.2590108914

C,0,1.2509711321,0.0301162077,1.9289804185
H,0,-0.8237552078,-0.2708257383,1.8080717141
C,0,2.5721881093,0.3482169504,1.272193441
H,0,1.2570978823,-0.1328746533,3.0059574816
H,0,3.1349093835,1.0548568778,1.8965134989
H,0,3.1878787255,-0.5642340932,1.2318031875
H,0,-0.6141218339,-0.7414692391,-0.6194135438
C,0,-0.8630556072,1.3799765932,-0.5768887444
C,0,1.3426807788,0.1050983975,-0.9241978757
H,0,-1.0594016273,1.4386372936,-1.653828054
H,0,-1.8287779559,1.3730882272,-0.058860909
H,0,-0.3349637829,2.2910888595,-0.2751816601
H,0,1.2519381268,0.4812841974,-1.9508138468
C,0,2.3839126992,0.919117283,-0.1414441465
H,0,1.6928077871,-0.933489512,-0.9996536222
H,0,3.3402855366,0.9299154574,-0.6774459988
H,0,2.05493238,1.9638449377,-0.0670161603

B3LYP/6-31G*
E(RB+HF-LYP) = -273.961823918

Zero-point correction= 0.175238 (Hartree/Particle)
Thermal correction to Energy= 0.182104
Thermal correction to Enthalpy= 0.183048
Thermal correction to Gibbs Free Energy= 0.144800
Sum of electronic and ZPE= -273.786586
Sum of electronic and thermal Energies= -273.779720
Sum of electronic and thermal Enthalpies= -273.778776
Sum of electronic and thermal Free Energies= -273.817024

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	114.272	26.825	80.500

C,0,-0.0422072968,0.1157988108,-0.2382926272
C,0,0.0945782337,-0.0624819274,1.2581984698
C,0,1.248611014,0.0308130031,1.9271501659
H,0,-0.824499851,-0.2754558828,1.8050684206
C,0,2.5696864018,0.3501080599,1.2717058417
H,0,1.2569088147,-0.1304651915,3.0048877428
H,0,3.1321782742,1.059247228,1.8947473656
H,0,3.1890698471,-0.5606400376,1.232387238
H,0,-0.6165318087,-0.7413728529,-0.622705303
C,0,-0.8588395686,1.3805582561,-0.5738937881

C,0,1.3421212843,0.1022057582,-0.9241186406
H,0,-1.0541759434,1.4444256008,-1.65126363
H,0,-1.8256737649,1.3753310689,-0.0565679514
H,0,-0.3282856271,2.2895991904,-0.268523164
H,0,1.2522650663,0.4759906074,-1.9522445204
C,0,2.3811452279,0.918802532,-0.1424168425
H,0,1.6932917405,-0.9365220618,-0.9969004574
H,0,3.338202919,0.9314898458,-0.6781501416
H,0,2.049383037,1.9630899926,-0.0693731781

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.168228	E(Thermal)=	0.175342
E(QCISD(T))=	-273.067221	E(Empiric)=	-0.135200
DE(Plus)=	-0.014054	DE(2DF)=	-0.257899
E(Delta-G3)=	-0.387011	E(G3-Empiric)=	-0.135200
G3(0 K)=	-273.693158	G3 Energy=	-273.686045
G3 Enthalpy=	-273.685100	G3 Free Energy=	-273.723765

CBS-QB3
C,0,-0.0405219203,0.1178639909,-0.2370983352
C,0,0.0965326268,-0.0613708748,1.2579208691
C,0,1.2476891573,0.0300891022,1.92464544
H,0,-0.8193763205,-0.2758321818,1.8045773422
C,0,2.5672844917,0.3511659458,1.2706598364
H,0,1.2553114707,-0.133531236,2.9994920787
H,0,3.1248140322,1.0600327403,1.8936082848
H,0,3.1856928562,-0.5572071846,1.2348404456
H,0,-0.6125323327,-0.7389819999,-0.61774989
C,0,-0.858151776,1.3805235067,-0.5733327084
C,0,1.3418111019,0.1037080207,-0.9240886735
H,0,-1.0531530755,1.4421795355,-1.6482819106
H,0,-1.8226762835,1.3735954898,-0.0572736025
H,0,-0.3300404518,2.2883347927,-0.2690323727
H,0,1.2507644198,0.4777317927,-1.9491045832
C,0,2.3817985657,0.9178197565,-0.1431122969
H,0,1.6905957032,-0.9331195575,-0.9979099256
H,0,3.3368493706,0.9264776373,-0.6770324498
H,0,2.0545363639,1.9610427235,-0.0720325483

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.171933	E(Thermal)=	0.178899
E(SCF)=	-272.137055	DE(MP2)=	-1.165868
DE(CBS)=	-0.109773	DE(MP34)=	-0.076098
DE(CCSD)=	-0.036504	DE(Int)=	0.039162

DE(Empirical)=	-0.058643		
CBS-QB3 (0 K)=	-273.372847	CBS-QB3 Energy=	-273.365880
CBS-QB3 Enthalpy=	-273.364936	CBS-QB3 Free Energy=	-273.403355

4e-3
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.619501849

Zero-point correction= 0.205860 (Hartree/Particle)
Thermal correction to Energy= 0.215101
Thermal correction to Enthalpy= 0.216045
Thermal correction to Gibbs Free Energy= 0.172738
Sum of electronic and ZPE= -300.413642
Sum of electronic and thermal Energies= -300.404401
Sum of electronic and thermal Enthalpies= -300.403457
Sum of electronic and thermal Free Energies= -300.446764

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.978	36.058	91.148

C,0,0.0214563126,0.0670460208,-0.1582826989
C,0,0.1930690026,-0.0440951408,1.3515986897
C,0,1.3923623201,0.111134392,1.9881448762
B,0,0.1935174985,1.7191286879,2.4243066868
H,0,-0.6462830419,-0.4566287047,1.905553982
C,0,2.6718230377,0.4371608168,1.2547922928
H,0,1.4875704068,-0.1989572786,3.0246721004
H,0,-0.2051291195,1.4092388383,3.511566538
H,0,-0.6443794202,2.0705349284,1.6392855319
H,0,1.1863297333,2.3941929061,2.3644344545
H,0,3.2604853935,1.157443642,1.8323634358
H,0,3.2662609183,-0.4890951629,1.2202274414
C,0,-0.8979600886,-1.0576939253,-0.6638972736
H,0,-0.4733225532,1.0217338148,-0.3742394675
C,0,1.3840949206,0.056598299,-0.8793409762
H,0,1.2461675814,0.3767908653,-1.9188158977
C,0,2.4161256779,0.9440653576,-0.1705133976
H,0,1.7624247265,-0.9757944488,-0.9172145432
H,0,3.3568339828,0.9634684101,-0.7322424453
H,0,2.0488988081,1.9770813837,-0.1284813042
H,0,-1.0327867083,-0.9845533818,-1.7484624897

H,0,-0.4740412703,-2.0452182161,-0.445106001
H,0,-1.8882461183,-1.0034221039,-0.1984015349

B3LYP/6-31G*
E(RB+HF-LYP) = -300.592165897

Zero-point correction= 0.207276 (Hartree/Particle)
Thermal correction to Energy= 0.216465
Thermal correction to Enthalpy= 0.217409
Thermal correction to Gibbs Free Energy= 0.174198
Sum of electronic and ZPE= -300.384890
Sum of electronic and thermal Energies= -300.375701
Sum of electronic and thermal Enthalpies= -300.374757
Sum of electronic and thermal Free Energies= -300.417968

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.834	35.764	90.945

C,0,0.0172590045,0.0673611676,-0.1578734716
C,0,0.1888466811,-0.0418873622,1.352015206
C,0,1.3877146544,0.1063975644,1.9884319064
B,0,0.202759742,1.7280233326,2.4176265688
H,0,-0.6537063954,-0.4492234252,1.9055878052
C,0,2.6683049201,0.4279032615,1.255264345
H,0,1.4820469882,-0.2038609791,3.0253725256
H,0,-0.2044840231,1.4197086753,3.5027327209
H,0,-0.6275340735,2.0868349314,1.6260349292
H,0,1.2038583609,2.3934154859,2.3652781788
H,0,3.2626943145,1.1409066842,1.8366743616
H,0,3.2586521584,-0.5011787047,1.2112398008
C,0,-0.8911783487,-1.0666447963,-0.6617362532
H,0,-0.485928918,1.0175253853,-0.3748100352
C,0,1.3795102966,0.0651967439,-0.8796734807
H,0,1.2406235741,0.3926787246,-1.9171998116
C,0,2.4105242574,0.9478162459,-0.1644146505
H,0,1.7600414358,-0.9663449582,-0.9261422457
H,0,3.3508680128,0.9745052292,-0.7274035564
H,0,2.0412116763,1.979865319,-0.1108525174
H,0,-1.0257466068,-0.9973437674,-1.7470896007
H,0,-0.458269129,-2.050207902,-0.4404293175
H,0,-1.8827965822,-1.0212868558,-0.1966854081

Temperature= 298.150000 Pressure= 1.000000

E(ZPE)=	0.198985	E(Thermal)=	0.208500
E(QCISD(T))=	-299.571436	E(Empiric)=	-0.155480
DE(Plus)=	-0.014468	DE(2DF)=	-0.299956
E(Delta-G3)=	-0.435949	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.278304	G3 Energy=	-300.268790
G3 Enthalpy=	-300.267845	G3 Free Energy=	-300.311649

CBS-QB3

C,0,0.0219697743,0.0655951897,-0.1570900685
C,0,0.1954108105,-0.0471676746,1.3500656685
C,0,1.3906053547,0.1043187187,1.984216159
B,0,0.1933663409,1.7310732441,2.4242247681
H,0,-0.6440048765,-0.4537800125,1.9039929458
C,0,2.6684267955,0.4319637785,1.2539860258
H,0,1.4829463248,-0.2014044672,3.0200172923
H,0,-0.1986347583,1.4173186573,3.5088350571
H,0,-0.6445323441,2.0748508142,1.6407351681
H,0,1.1873011844,2.3979882478,2.3609369457
H,0,3.2543643221,1.1499332532,1.8330470841
H,0,3.2639168808,-0.4913533351,1.2179758795
C,0,-0.8934738638,-1.0599441439,-0.6632846915
H,0,-0.4745129033,1.0177252848,-0.3687563449
C,0,1.3821523176,0.0595044636,-0.879451898
H,0,1.243447358,0.3844515958,-1.914942874
C,0,2.413719869,0.9425445189,-0.1682768659
H,0,1.7596394208,-0.9707104187,-0.9228511277
H,0,3.3524781682,0.9630511505,-0.7289025611
H,0,2.0481644819,1.9737458327,-0.1231920694
H,0,-1.027665665,-0.9870880031,-1.7458833323
H,0,-0.4676072337,-2.0444075903,-0.4444600866

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203193	E(Thermal)=	0.212562
E(SCF)=	-298.533335	DE(MP2)=	-1.303099
DE(CBS)=	-0.122884	DE(MP34)=	-0.092663
DE(CCSD)=	-0.041055	DE(Int)=	0.044552
DE(Empirical)=	-0.066826		
CBS-QB3 (0 K)=	-299.912117	CBS-QB3 Energy=	-299.902749
CBS-QB3 Enthalpy=	-299.901804	CBS-QB3 Free Energy=	-299.945397

4e-4

B3LYP/6-31+G**

E(RB+HF-LYP) = -300.618237874

Zero-point correction= 0.205705 (Hartree/Particle)
Thermal correction to Energy= 0.215048
Thermal correction to Enthalpy= 0.215992
Thermal correction to Gibbs Free Energy= 0.172186
Sum of electronic and ZPE= -300.412533
Sum of electronic and thermal Energies= -300.403190
Sum of electronic and thermal Enthalpies= -300.402246
Sum of electronic and thermal Free Energies= -300.446052

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.944	36.123	92.197

C,0,-0.0253107827,0.1031813629,-0.1909933473
C,0,0.1130122148,-0.0274012811,1.3151989208
C,0,1.3118139371,0.0982823976,1.9653211545
B,0,0.1347068418,1.7015744972,2.3761805675
H,0,-0.7360256534,-0.4387274358,1.853067933
C,0,2.6214722153,0.3580758886,1.2443699291
H,0,1.3889539935,-0.2273630659,2.9992448077
H,0,-0.232886735,1.4195922029,3.4819674861
H,0,-0.7335764937,2.032828849,1.6147342041
H,0,1.0969471307,2.4117500897,2.2700578865
C,0,3.6339703664,1.1640802429,2.0699170659
H,0,3.0547657049,-0.6483906919,1.1072311962
H,0,-0.6284021569,-0.7422751966,-0.5454958389
H,0,-0.6011357675,1.0039684607,-0.4285333782
C,0,1.3316937555,0.1238365719,-0.9196778383
H,0,1.1988700257,0.5156780967,-1.9342777238
C,0,2.377615826,0.9465213704,-0.1543508456
H,0,1.7027266621,-0.9044914158,-1.0287602933
H,0,3.3232484347,0.9719301205,-0.7089301442
H,0,2.0383690017,1.9857961678,-0.0530921853
H,0,4.605369712,1.1832389087,1.5639491968
H,0,3.3002582116,2.1956318715,2.2113758976
H,0,3.7813455553,0.7197449881,3.0609473491

B3LYP/6-31G*
E(RB+HF-LYP) = -300.591119710

Zero-point correction= 0.207176 (Hartree/Particle)
Thermal correction to Energy= 0.216440

Thermal correction to Enthalpy= 0.217384
Thermal correction to Gibbs Free Energy= 0.173797
Sum of electronic and ZPE= -300.383944
Sum of electronic and thermal Energies= -300.374680
Sum of electronic and thermal Enthalpies= -300.373736
Sum of electronic and thermal Free Energies= -300.417322

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.818	35.804	91.740

C,0,-0.0254885296,0.1003739862,-0.1895391358
C,0,0.1139059489,-0.0284504463,1.3167696661
C,0,1.3121998009,0.095364111,1.9657293922
B,0,0.1384637865,1.7065201564,2.3697194871
H,0,-0.7360901224,-0.4382196728,1.8550548353
C,0,2.6215002414,0.355039923,1.2445920617
H,0,1.3904264538,-0.2288046974,3.0003447145
H,0,-0.2293771868,1.4250772423,3.4759953433
H,0,-0.7294233652,2.038187447,1.6060966521
H,0,1.1033040755,2.4151985008,2.2636559212
C,0,3.6319970192,1.1612946324,2.0713392249
H,0,3.0568093388,-0.6505037247,1.1037906854
H,0,-0.6261106771,-0.7472422409,-0.5449467607
H,0,-0.6045751791,0.9993395995,-0.4270401176
C,0,1.3311637068,0.1250402074,-0.9180285809
H,0,1.1973685043,0.5178529492,-1.9326087608
C,0,2.3751780045,0.9480837943,-0.1515252092
H,0,1.7040350905,-0.9027847463,-1.0288748709
H,0,3.3204555452,0.9786924559,-0.7073811985
H,0,2.032619947,1.9860987506,-0.0459403805
H,0,4.6019555282,1.1902142354,1.5618242259
H,0,3.2915976603,2.1898300801,2.2211281623
H,0,3.7858864081,0.7108604569,3.0592966429

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.198888	E(Thermal)=	0.208477
E(QCISD(T))=	-299.570386	E(Empiric)=	-0.155480
DE(Plus)=	-0.014056	DE(2DF)=	-0.299966
E(Delta-G3)=	-0.436266	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.277266	G3 Energy=	-300.267677
G3 Enthalpy=	-300.266733	G3 Free Energy=	-300.310915

CBS-QB3

C,0,-0.0218684361,0.1060074643,-0.1897963691
C,0,0.117333518,-0.0308973472,1.3131790235
C,0,1.3120701333,0.0912143537,1.961158004
B,0,0.1359905465,1.7114499608,2.3744144789
H,0,-0.7307615383,-0.4399215741,1.8498079316
C,0,2.6207306214,0.3544877847,1.244482413
H,0,1.3868259873,-0.2335058615,2.9931864638
H,0,-0.1991442872,1.4323343716,3.4872650528
H,0,-0.7547658956,2.0167709734,1.6329828104
H,0,1.086532319,2.4255581343,2.2354309592
C,0,3.6270793657,1.1626131673,2.072455179
H,0,3.0565724336,-0.6487783565,1.1076911077
H,0,-0.6277001851,-0.7335292295,-0.5473435302
H,0,-0.5933792032,1.0083794566,-0.4217256629
C,0,1.3331149373,0.1246065418,-0.9184507413
H,0,1.2011444174,0.5175391942,-1.9303081299
C,0,2.3795946828,0.9430548265,-0.1530028184
H,0,1.7005362222,-0.9025781354,-1.0289946677
H,0,3.3236657203,0.9662580246,-0.7059094219
H,0,2.0433970067,1.9810525349,-0.0519088857
H,0,4.5962057228,1.1914539087,1.566795672
H,0,3.2861931169,2.1888320509,2.2190379799

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203080	E(Thermal)=	0.212537
E(SCF)=	-298.530266	DE(MP2)=	-1.305055
DE(CBS)=	-0.123037	DE(MP34)=	-0.092458
DE(CCSD)=	-0.041148	DE(Int)=	0.044569
DE(Empirical)=	-0.066815		
CBS-QB3 (0 K)=	-299.911129	CBS-QB3 Energy=	-299.901672
CBS-QB3 Enthalpy=	-299.900728	CBS-QB3 Free Energy=	-299.944809

4e-5
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.617754492

Zero-point correction= 0.206014 (Hartree/Particle)
Thermal correction to Energy= 0.215331
Thermal correction to Enthalpy= 0.216275
Thermal correction to Gibbs Free Energy= 0.172752
Sum of electronic and ZPE= -300.411740
Sum of electronic and thermal Energies= -300.402423
Sum of electronic and thermal Enthalpies= -300.401479

Sum of electronic and thermal Free Energies= -300.445003

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.122	36.063	91.603

C,0,-0.2744162381,0.3588854602,-0.0851019511
C,0,-0.2430148795,0.4379823144,1.428518549
C,0,0.8879176859,0.7287995505,2.1379333875
B,0,-0.3926315746,2.3377269162,2.256769134
H,0,-1.1172324023,0.070990347,1.9586381048
C,0,2.2298638711,1.0131740353,1.4915317626
H,0,0.8973479486,0.5587613385,3.2110351406
H,0,-0.8508963598,2.1598428539,3.3500638355
H,0,-1.1918547348,2.5205809614,1.3795003801
H,0,0.5699554222,3.0494806308,2.1592258294
H,0,2.6632236828,1.8871882036,1.9923884928
C,0,3.1835953429,-0.1740572221,1.7451552315
H,0,-0.8202394542,-0.5523373298,-0.3612193075
H,0,-0.8630297577,1.193234473,-0.4821602837
C,0,1.1318948281,0.3464047619,-0.7103988173
H,0,1.0630413619,0.5788926043,-1.7788699194
C,0,2.0642231575,1.3428345065,-0.0060384839
H,0,1.5535997654,-0.6642648814,-0.6410560301
H,0,3.048410661,1.3543859448,-0.4892627207
H,0,1.6498009111,2.3539485232,-0.1016878669
H,0,4.1826405372,0.0535903808,1.3576195908
H,0,3.2809473386,-0.3816857847,2.8166417574
H,0,2.8328318868,-1.0915305882,1.2610511849

B3LYP/6-31G*
E(RB+HF-LYP) = -300.590579335

Zero-point correction= 0.207403 (Hartree/Particle)
Thermal correction to Energy= 0.216687
Thermal correction to Enthalpy= 0.217631
Thermal correction to Gibbs Free Energy= 0.174124
Sum of electronic and ZPE= -300.383176
Sum of electronic and thermal Energies= -300.373892
Sum of electronic and thermal Enthalpies= -300.372948
Sum of electronic and thermal Free Energies= -300.416455

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 135.973 35.780 91.568

C,0,-0.0773729778,0.1629930523,-0.2115996458
C,0,0.0747637073,-0.0061420476,1.2872820975
C,0,1.2787732339,0.0524982154,1.9275522018
B,0,0.2034599569,1.7506483191,2.3988318582
H,0,-0.7951832083,-0.3632374748,1.8317745543
C,0,2.5928343555,0.3016460183,1.2138055998
H,0,1.348199653,-0.2861853922,2.9580402614
H,0,-0.2029400166,1.4434056492,3.4844623919
H,0,-0.6206862808,2.1582291591,1.6249840566
H,0,1.2390039278,2.3584794742,2.3377292433
H,0,3.1619255314,1.0296865916,1.804763979
C,0,3.4165947515,-1.0030052838,1.1848412516
H,0,-0.7350981188,-0.6375247726,-0.5754940759
H,0,-0.603466198,1.1012641612,-0.4203744662
C,0,1.2691329327,0.1225636289,-0.9556897472
H,0,1.1468802537,0.5358719801,-1.963475023
C,0,2.3540026058,0.8928680933,-0.1899284633
H,0,1.5827483331,-0.9212344977,-1.0866277858
H,0,3.294874677,0.8918255582,-0.7539330927
H,0,2.0459995764,1.9406225354,-0.083520281
H,0,4.40256139,-0.8190249905,0.7430157351
H,0,3.5719218746,-1.3962977427,2.1963689846
H,0,2.92300204,-1.7856622345,0.5982973661

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.199107 E(Thermal)= 0.208714
E(QCISD(T))= -299.570000 E(Empiric)= -0.155480
DE(Plus)= -0.014284 DE(2DF)= -0.300131
E(Delta-G3)= -0.436105 E(G3-Empiric)= -0.155480
G3(0 K)= -300.276892 G3 Energy= -300.267285
G3 Enthalpy= -300.266341 G3 Free Energy= -300.310441

CBS-QB3

C,0,-0.2333295042,0.3679822321,-0.1238011247
C,0,-0.2425969298,0.4162904728,1.3886671616
C,0,0.8618207069,0.7022996326,2.131582072
B,0,-0.4405784617,2.3036211256,2.2546696402
H,0,-1.1259223617,0.0323410947,1.8860546496
C,0,2.2161528697,1.010522597,1.5267804644
H,0,0.8437252778,0.5147569158,3.1995294731
H,0,-0.9642916826,2.0786282956,3.3052190741
H,0,-1.1727467126,2.5292643573,1.3348046529

H,0,0.5315780652,3.004445165,2.2569358887
H,0,2.6285223179,1.8665872879,2.0658824719
C,0,3.1724751684,-0.2004131961,1.7464336298
H,0,-0.7457939399,-0.5499785481,-0.4319519353
H,0,-0.8339051632,1.1926748318,-0.5170961722
C,0,1.1862570165,0.4069185981,-0.7127487357
H,0,1.1390046354,0.6645677379,-1.7742466808
C,0,2.0730409657,1.4027751059,0.0438663568
H,0,1.6313918895,-0.5930138411,-0.6567073977
H,0,3.0645571023,1.4621854761,-0.4147689737
H,0,1.6317085983,2.4027507868,-0.0187263447
H,0,3.5787164181,-0.5592712546,0.7976467438
H,0,4.0166360008,0.0741485224,2.3823720007

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.202926	E(Thermal)=	0.211832
E(SCF)=	-298.526339	DE(MP2)=	-1.304120
DE(CBS)=	-0.122918	DE(MP34)=	-0.092682
DE(CCSD)=	-0.041125	DE(Int)=	0.044575
DE(Empirical)=	-0.066815		
CBS-QB3 (0 K)=	-299.906498	CBS-QB3 Energy=	-299.897592
CBS-QB3 Enthalpy=	-299.896648	CBS-QB3 Free Energy=	-299.939567

4e-6
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.616076432

Zero-point correction= 0.206308 (Hartree/Particle)
Thermal correction to Energy= 0.215330
Thermal correction to Enthalpy= 0.216274
Thermal correction to Gibbs Free Energy= 0.173536
Sum of electronic and ZPE= -300.409768
Sum of electronic and thermal Energies= -300.400747
Sum of electronic and thermal Enthalpies= -300.399803
Sum of electronic and thermal Free Energies= -300.442540

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.121	35.725	89.949

C,0,-0.2234187211,0.4150454924,-0.0825847225
C,0,-0.2230728446,0.5290428889,1.4368307487

C,0,0.9074695117,0.7158636534,2.1883352581
B,0,-0.2372838449,2.3499294716,2.3605279313
H,0,-1.1334174795,0.2033238075,1.9333203522
C,0,2.2621376939,0.9490962581,1.5601311621
H,0,0.8878255383,0.4831744915,3.2485861013
H,0,-0.8074195967,2.1442569838,3.3952085164
H,0,-0.9337517668,2.7062141966,1.450958581
H,0,0.778087422,2.9924051071,2.4037424678
H,0,2.8278281406,1.6752089214,2.152733552
H,0,2.8201246876,0.0014235399,1.6137913311
H,0,-0.6297989216,-0.5930226079,-0.2583810458
C,0,-1.1745192834,1.3886228995,-0.8007888082
C,0,1.211271044,0.4450115185,-0.6669576856
H,0,1.1657258573,0.7186845576,-1.7273455554
C,0,2.141024163,1.3961376416,0.0986001483
H,0,1.6395345255,-0.5657037529,-0.6252157169
H,0,3.1312698844,1.4189195685,-0.3699979276
H,0,1.7478961779,2.4196375227,0.0639658041
H,0,-1.293583516,1.0852410336,-1.8467134996
H,0,-2.1643864815,1.4015620684,-0.333511947
H,0,-0.78709719,2.4112157382,-0.7805600458

B3LYP/6-31G*
E(RB+HF-LYP) = -300.589001468

Zero-point correction= 0.207700 (Hartree/Particle)
Thermal correction to Energy= 0.216689
Thermal correction to Enthalpy= 0.217634
Thermal correction to Gibbs Free Energy= 0.174932
Sum of electronic and ZPE= -300.381301
Sum of electronic and thermal Energies= -300.372312
Sum of electronic and thermal Enthalpies= -300.371368
Sum of electronic and thermal Free Energies= -300.414070

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.974	35.444	89.878

C,0,-0.2238560693,0.4121199379,-0.0822361633
C,0,-0.2228060361,0.5249937912,1.4371003314
C,0,0.9064823359,0.7132272353,2.1876983712
B,0,-0.2364355384,2.3539760553,2.3566940047
H,0,-1.1334504041,0.1986308608,1.933233586
C,0,2.2607918955,0.9486215197,1.5600693158

H,0,0.887984945,0.4821022374,3.2486711536
H,0,-0.803605621,2.145575578,3.3929541184
H,0,-0.9369096855,2.7063585501,1.4471659435
H,0,0.7804757333,2.9962023959,2.3969787348
H,0,2.8248300201,1.6765105339,2.1527879489
H,0,2.8225778009,0.0025776021,1.6133300978
H,0,-0.6316142469,-0.5951388208,-0.2625117768
C,0,-1.171649587,1.390166577,-0.7972056785
C,0,1.2108797511,0.4430060425,-0.666067257
H,0,1.1659810172,0.715584703,-1.7272380763
C,0,2.1378856985,1.3960281321,0.0992700772
H,0,1.6405488661,-0.5674185024,-0.6232571501
H,0,3.1282702187,1.4225835306,-0.3699861828
H,0,1.7409574654,2.4184687483,0.0662834462
H,0,-1.289194491,1.0925536872,-1.8456637286
H,0,-2.1631270687,1.40220136,-0.33215647
H,0,-0.7825719997,2.4123592449,-0.7712396459

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199391	E(Thermal)=	0.208709
E(QCISD(T))=	-299.568326	E(Empiric)=	-0.155480
DE(Plus)=	-0.014040	DE(2DF)=	-0.300446
E(Delta-G3)=	-0.436359	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.275260	G3 Energy=	-300.265941
G3 Enthalpy=	-300.264997	G3 Free Energy=	-300.308288

CBS-QB3

C,0,-0.2217433205,0.4137072562,-0.0824054145
C,0,-0.220246943,0.5246015944,1.4350050938
C,0,0.9062196254,0.7108091078,2.1836909873
B,0,-0.2393576435,2.3597619249,2.3609292592
H,0,-1.128978714,0.2012458318,1.9313749941
C,0,2.2587451026,0.9481917801,1.5585169134
H,0,0.8848825332,0.4822442029,3.2425478946
H,0,-0.8017026059,2.1471966154,3.394257631
H,0,-0.9387696355,2.7080405903,1.4547786159
H,0,0.7760430443,2.996136407,2.4005171537
H,0,2.8194356915,1.6749963965,2.1509312421
H,0,2.8199521393,0.0046940401,1.6137915167
H,0,-0.6274008488,-0.591987832,-0.2606929705
C,0,-1.1705437373,1.3890643631,-0.7972716175
C,0,1.2111259045,0.443709712,-0.6666706427
H,0,1.1653537734,0.7169845876,-1.7247296892
C,0,2.1388636135,1.3942406196,0.0984651383

H,0,1.6383089746,-0.5650977567,-0.6251435088
H,0,3.1274111199,1.4177003911,-0.3684493586
H,0,1.7460111316,2.4155552827,0.0632724242
H,0,-1.2861415602,1.0914164256,-1.8432629959
H,0,-2.1601974341,1.3981707147,-0.3342374974

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203632	E(Thermal)=	0.212791
E(SCF)=	-298.527656	DE(MP2)=	-1.306304
DE(CBS)=	-0.123091	DE(MP34)=	-0.092210
DE(CCSD)=	-0.041212	DE(Int)=	0.044581
DE(Empirical)=	-0.066797		
CBS-QB3 (0 K)=	-299.909058	CBS-QB3 Energy=	-299.899898
CBS-QB3 Enthalpy=	-299.898954	CBS-QB3 Free Energy=	-299.941984

4e-7
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.614982021

Zero-point correction= 0.206017 (Hartree/Particle)
Thermal correction to Energy= 0.214174
Thermal correction to Enthalpy= 0.215118
Thermal correction to Gibbs Free Energy= 0.174088
Sum of electronic and ZPE= -300.408965
Sum of electronic and thermal Energies= -300.400808
Sum of electronic and thermal Enthalpies= -300.399864
Sum of electronic and thermal Free Energies= -300.440894

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.396	33.208	86.356

C,0,2.2744773466,0.6161794655,1.2189324859
H,0,2.730270376,-0.1890787995,1.7902178078
C,0,1.1057335366,1.2221594482,1.7462394924
C,0,0.0509130696,1.8906797972,0.8438303472
C,0,0.2767152645,1.5604679899,-0.645882304
C,0,1.7554592168,1.6461710544,-1.0449723405
C,0,2.572972127,0.606039823,-0.2685449592
H,0,2.3000785268,-0.4006713557,-0.6191487173
B,0,2.4931685247,2.1756413917,2.193670814
H,0,0.1325163421,2.9779237092,0.9588659129

C,0,-1.3615139491,1.4847213912,1.2903747584
H,0,-0.0871329137,0.5413300562,-0.8484219524
H,0,-0.328299939,2.2355990525,-1.2631770358
H,0,2.1409681332,2.6520406219,-0.8406452923
H,0,1.8749676454,1.4716743582,-2.1204447686
H,0,3.6468936195,0.718478624,-0.4518513411
H,0,3.5053660707,1.664230709,1.6898429859
H,0,2.3932592174,3.2337600674,1.6455113558
H,0,2.6690229657,2.0675603393,3.3728098383
H,0,0.7125255657,0.7879639469,2.6613494894
H,0,-1.5484587836,1.7761755672,2.3300250131
H,0,-2.1214854927,1.9679581418,0.6657889636
H,0,-1.5041534702,0.3996206005,1.2132504466

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.199192 E(Thermal)= 0.207588
E(QCISD(T))= -299.566480 E(Empiric)= -0.155480
DE(Plus)= -0.014602 DE(2DF)= -0.301105
E(Delta-G3)= -0.435295 E(G3-Empiric)= -0.155480
G3(0 K)= -300.273770 G3 Energy= -300.265373
G3 Enthalpy= -300.264429 G3 Free Energy= -300.305860

CBS-QB3

C,0,2.2733674188,0.6182659249,1.2192542854
H,0,2.7262748678,-0.1858144094,1.7897894882
C,0,1.1064077912,1.2237551877,1.7456221864
C,0,0.0517239235,1.8904882311,0.8443906049
C,0,0.2776795492,1.5626077915,-0.6441782984
C,0,1.755077729,1.6465944955,-1.0419467263
C,0,2.5699504432,0.6064763929,-0.2662264409
H,0,2.2961499514,-0.3980868259,-0.6164835573
B,0,2.4901579063,2.1776017523,2.1906660537
H,0,0.1326076928,2.9752077095,0.9609926607
C,0,-1.3586382426,1.4818625152,1.2892077809
H,0,-0.0869928949,0.5463043532,-0.847874466
H,0,-0.3245402615,2.2382570644,-1.2595974413
H,0,2.140904673,2.6500426638,-0.8379713929
H,0,1.8744939543,1.4726583791,-2.1152838754
H,0,3.6417968953,0.716541179,-0.4496855005
H,0,3.5012789356,1.6581096063,1.6899390365
H,0,2.397765228,3.2301679373,1.6386774818
H,0,2.6669242923,2.0724226055,3.3662818649
H,0,0.7139286218,0.789566965,2.6579505733
H,0,-1.5458147799,1.7714771694,2.3271756829

H,0,-2.1178516138,1.9635926676,0.6660794297

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203403	E(Thermal)=	0.211647
E(SCF)=	-298.517215	DE(MP2)=	-1.316243
DE(CBS)=	-0.123986	DE(MP34)=	-0.089923
DE(CCSD)=	-0.041491	DE(Int)=	0.044679
DE(Empirical)=	-0.066746		
CBS-QB3 (0 K)=	-299.907522	CBS-QB3 Energy=	-299.899278
CBS-QB3 Enthalpy=	-299.898334	CBS-QB3 Free Energy=	-299.939519

4e-8
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.614928509

Zero-point correction= 0.206032 (Hartree/Particle)
Thermal correction to Energy= 0.214183
Thermal correction to Enthalpy= 0.215127
Thermal correction to Gibbs Free Energy= 0.174044
Sum of electronic and ZPE= -300.408896
Sum of electronic and thermal Energies= -300.400746
Sum of electronic and thermal Enthalpies= -300.399802
Sum of electronic and thermal Free Energies= -300.440884

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.402	33.106	86.466

C,0,0.0364091868,0.1342888749,-0.127687292
C,0,0.1669270457,-0.0017467306,1.3972830467
C,0,1.393370616,0.2215051039,2.0799249184
B,0,0.3368047762,1.5461578808,2.3974909061
H,0,-0.5594246281,-0.657474832,1.8723765764
C,0,2.6840233666,0.5081009909,1.3192589474
H,0,1.5301793577,-0.3301544367,3.0062424539
H,0,0.0594691676,1.5312620486,3.561983309
H,0,-0.7542156814,1.3214518994,1.8475294556
H,0,0.7537740839,2.5121636871,1.8234063124
H,0,3.2744795515,1.2646072366,1.8477662964
H,0,3.2835227517,-0.4144146958,1.3258172796
C,0,-0.9707119068,-0.8914262604,-0.6669546951
H,0,-0.3462181041,1.1366103974,-0.3538080461

C,0,1.4152728921,0.0122310096,-0.8048542214
H,0,1.3108490691,0.2536164508,-1.8696227483
C,0,2.4472388006,0.9294668836,-0.13750466
H,0,1.7600534052,-1.0312040933,-0.7504583728
H,0,3.3959683293,0.9026536183,-0.685976456
H,0,2.089922734,1.9661778462,-0.1740776501
H,0,-1.0734973945,-0.7978338718,-1.7532081585
H,0,-0.6463180291,-1.9164300635,-0.4499082137
H,0,-1.9626073898,-0.749448944,-0.2230699879

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199179	E(Thermal)=	0.207581
E(QCISD(T))=	-299.566611	E(Empiric)=	-0.155480
DE(Plus)=	-0.014556	DE(2DF)=	-0.300928
E(Delta-G3)=	-0.435310	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.273706	G3 Energy=	-300.265304
G3 Enthalpy=	-300.264359	G3 Free Energy=	-300.305882

CBS-QB3

C,0,0.0368663725,0.1348410597,-0.126513967
C,0,0.1674859535,0.0006734272,1.3967499441
C,0,1.392379229,0.2215419218,2.07820907
B,0,0.3397262865,1.5465733443,2.395807233
H,0,-0.5569743524,-0.6532391878,1.8711807203
C,0,2.6815748919,0.5058288532,1.3183094769
H,0,1.5279129376,-0.3297538328,3.0019722032
H,0,0.0609746105,1.5315192811,3.556332098
H,0,-0.7513675008,1.3188742694,1.8448019068
H,0,0.751879303,2.5100217548,1.8217384496
H,0,3.2720676443,1.2593418236,1.8464727811
H,0,3.2792792125,-0.4155062493,1.3238452296
C,0,-0.9676163464,-0.8913384274,-0.6650418184
H,0,-0.345879627,1.1348716518,-0.3510545238
C,0,1.4139202263,0.0140027225,-0.8038423712
H,0,1.3095752735,0.2569917117,-1.8659487633
C,0,2.4450355486,0.9289083325,-0.1360205596
H,0,1.7579756506,-1.0275662137,-0.7516523266
H,0,3.3917593069,0.9027819918,-0.6835659725
H,0,2.088868638,1.9637885276,-0.1708665869
H,0,-1.0687368405,-0.799988513,-1.7496270821
H,0,-0.6430378338,-1.9136561535,-0.4456975055

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)=	0.203425	E(Thermal)=	0.211660
E(SCF)=	-298.516686	DE(MP2)=	-1.316657
DE(CBS)=	-0.124084	DE(MP34)=	-0.089936
DE(CCSD)=	-0.041496	DE(Int)=	0.044690
DE(Empirical)=	-0.066742		
CBS-QB3 (0 K)=	-299.907486	CBS-QB3 Energy=	-299.899252
CBS-QB3 Enthalpy=	-299.898308	CBS-QB3 Free Energy=	-299.939541

4e-9
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.614780437

Zero-point correction= 0.205989 (Hartree/Particle)
Thermal correction to Energy= 0.214149
Thermal correction to Enthalpy= 0.215093
Thermal correction to Gibbs Free Energy= 0.174137
Sum of electronic and ZPE= -300.408791
Sum of electronic and thermal Energies= -300.400631
Sum of electronic and thermal Enthalpies= -300.399687
Sum of electronic and thermal Free Energies= -300.440643

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.381	33.195	86.199

C,0,-0.044626164,0.2702722535,-0.1746436233
C,0,0.0498694359,0.0612730452,1.337676847
C,0,1.2854677478,0.169809078,2.029339551
B,0,0.3262365406,1.5629688636,2.3858075752
H,0,-0.7274512247,-0.5520790579,1.7855180803
C,0,2.6113869649,0.3691179975,1.2909312323
H,0,1.3752181432,-0.4144505072,2.9422329124
H,0,0.0594131213,1.5341048938,3.5524927883
H,0,-0.7797772232,1.4392786135,1.841539945
H,0,0.8045743421,2.5142733688,1.8368531234
C,0,3.6142937569,1.2039259302,2.0976633133
H,0,3.0409522764,-0.6413951801,1.1861029771
H,0,-0.76182763,-0.4553464493,-0.5752575425
H,0,-0.4550266548,1.2619621166,-0.3910732647
C,0,1.3192857674,0.1212761175,-0.8711328867
H,0,1.2322155347,0.4547027794,-1.9117481473
C,0,2.4063806478,0.9115349595,-0.132785365

H,0,1.6039043812,-0.9396108431,-0.9042551242
H,0,3.356195546,0.8556761673,-0.678671126
H,0,2.1285481396,1.972789663,-0.0891878472
H,0,4.5867822312,1.2367836414,1.5927159918
H,0,3.2564280209,2.2306863491,2.2231057662
H,0,3.7693582988,0.7795091998,3.0962258237

B3LYP/6-31G*
E(RB+HF-LYP) = -300.586967276

Zero-point correction= 0.207448 (Hartree/Particle)
Thermal correction to Energy= 0.215538
Thermal correction to Enthalpy= 0.216482
Thermal correction to Gibbs Free Energy= 0.175642
Sum of electronic and ZPE= -300.379519
Sum of electronic and thermal Energies= -300.371429
Sum of electronic and thermal Enthalpies= -300.370485
Sum of electronic and thermal Free Energies= -300.411326

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.252	32.820	85.956

C,0,-0.0447709171,0.2748547013,-0.1742933951
C,0,0.0482431047,0.064816339,1.3387127407
C,0,1.2856911281,0.1751919583,2.0325903063
B,0,0.3353679036,1.5625264758,2.3866685777
H,0,-0.7246852042,-0.5581759331,1.7824486338
C,0,2.6112482793,0.3677178852,1.2918944347
H,0,1.3754158245,-0.4188225694,2.9397668939
H,0,0.0576474943,1.5387656861,3.5516012173
H,0,-0.7744696381,1.4231007806,1.8398291362
H,0,0.7953924426,2.5193115313,1.8296355413
C,0,3.6137470204,1.2035135652,2.0968992143
H,0,3.0404716026,-0.6431970873,1.1859052704
H,0,-0.7656344576,-0.4462308158,-0.5776676175
H,0,-0.4492063454,1.2693555134,-0.3904041458
C,0,1.3190767744,0.1200935563,-0.8683659438
H,0,1.2334549912,0.4496834564,-1.9108352187
C,0,2.4059534718,0.9107624445,-0.1312023458
H,0,1.6012122462,-0.9418802045,-0.8973957327
H,0,3.3557453832,0.8557873636,-0.6781633916
H,0,2.1271867346,1.9720803183,-0.0878971466
H,0,4.585476066,1.2412633788,1.5895223011

H,0,3.2521495363,2.2290209143,2.2254692096
H,0,3.7730885586,0.7775237418,3.0947334603

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199150	E(Thermal)=	0.207555
E(QCISD(T))=	-299.567059	E(Empiric)=	-0.155480
DE(Plus)=	-0.014301	DE(2DF)=	-0.300777
E(Delta-G3)=	-0.435599	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.274066	G3 Energy=	-300.265661
G3 Enthalpy=	-300.264717	G3 Free Energy=	-300.306093

CBS-QB3
C,0,-0.0426094038,0.2705629932,-0.1724149399
C,0,0.0518891456,0.0632507683,1.3379082409
C,0,1.2857520119,0.1700990911,2.0283379438
B,0,0.3299506829,1.5636198786,2.383803682
H,0,-0.7232396811,-0.548889866,1.7848469083
C,0,2.6102698725,0.3681059132,1.2908874544
H,0,1.3742161523,-0.4135354455,2.9388254848
H,0,0.0626121176,1.5363053206,3.5467721161
H,0,-0.7767067392,1.4351756257,1.8399532434
H,0,0.8015969771,2.5126311732,1.8329960945
C,0,3.6113527034,1.2027081842,2.0968091749
H,0,3.0390135643,-0.6404199398,1.1858901496
H,0,-0.7578637853,-0.4542741507,-0.5721464678
H,0,-0.4535360657,1.2597472907,-0.3878437707
C,0,1.3194565317,0.1226204969,-0.8689611973
H,0,1.2322524169,0.4567919849,-1.9069793157
C,0,2.4057229972,0.9108788326,-0.1310052089
H,0,1.6033189312,-0.9362058777,-0.903759002
H,0,3.353475108,0.8550348477,-0.6759884124
H,0,2.1290110502,1.970166349,-0.0863892429
H,0,4.5814483816,1.2382397365,1.591723547
H,0,3.2520840232,2.2266670473,2.223554073

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203373	E(Thermal)=	0.211620
E(SCF)=	-298.516213	DE(MP2)=	-1.317543
DE(CBS)=	-0.124169	DE(MP34)=	-0.089734
DE(CCSD)=	-0.041552	DE(Int)=	0.044710
DE(Empirical)=	-0.066735		
CBS-QB3 (0 K)=	-299.907861	CBS-QB3 Energy=	-299.899614
CBS-QB3 Enthalpy=	-299.898670	CBS-QB3 Free Energy=	-299.939779

4e-10
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.614955673

Zero-point correction= 0.206087 (Hartree/Particle)
Thermal correction to Energy= 0.214214
Thermal correction to Enthalpy= 0.215158
Thermal correction to Gibbs Free Energy= 0.174290
Sum of electronic and ZPE= -300.408868
Sum of electronic and thermal Energies= -300.400742
Sum of electronic and thermal Enthalpies= -300.399797
Sum of electronic and thermal Free Energies= -300.440666

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.421	33.197	86.015

C,0,2.2552262768,0.628626149,1.1505811612
H,0,2.7767082095,-0.1437767428,1.7125418543
C,0,1.0449717708,1.1310572052,1.6872988365
C,0,-0.0364954354,1.7423859393,0.787701231
C,0,0.2143296504,1.4988780374,-0.7121437835
C,0,1.6928318851,1.6766640828,-1.0837396494
C,0,2.5705011916,0.6581017443,-0.3379422312
H,0,2.2642518138,-0.346004348,-0.6781245171
B,0,2.3544883479,2.1800417021,2.165404318
H,0,-0.1206592118,2.817044934,0.9789045051
H,0,-1.0022030936,1.3050453148,1.0679178616
H,0,-0.0907417096,0.475583358,-0.9738553755
H,0,-0.4137913884,2.1719329526,-1.3070655957
H,0,2.0244026665,2.694520386,-0.8419115155
H,0,1.8345412257,1.5446617128,-2.1632907659
C,0,4.0645058202,0.808414885,-0.6504672319
H,0,3.412599744,1.7852154301,1.65533308
H,0,2.154588838,3.2419350504,1.6528743864
H,0,2.5319700581,2.0528222165,3.3427277468
H,0,0.6813110793,0.6488368078,2.5894596136
H,0,4.2475631011,0.6672680801,-1.7210298971
H,0,4.4258067025,1.8044193876,-0.3736919455
H,0,4.6638984575,0.0686297149,-0.1073520861

Temperature= 298.150000 Pressure= 1.000000

E(ZPE)=	0.199255	E(Thermal)=	0.207621
E(QCISD(T))=	-299.566779	E(Empiric)=	-0.155480
DE(Plus)=	-0.014242	DE(2DF)=	-0.300944
E(Delta-G3)=	-0.435639	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.273828	G3 Energy=	-300.265462
G3 Enthalpy=	-300.264518	G3 Free Energy=	-300.305793

CBS-QB3

C,0,2.255354169,0.6301786465,1.1502260288
H,0,2.7728436663,-0.1425451207,1.7107584293
C,0,1.0466633806,1.1321696298,1.6862612826
C,0,-0.0339579819,1.7418864429,0.7875673863
C,0,0.2160079214,1.4983300265,-0.7105771978
C,0,1.6926941251,1.6758202355,-1.0821226916
C,0,2.569622545,0.6588476482,-0.3364308123
H,0,2.2645078407,-0.3434658033,-0.6765532698
B,0,2.3515992049,2.1802029132,2.1621027333
H,0,-0.1177921627,2.8143338077,0.978445364
H,0,-0.9977705493,1.3056483498,1.0676164774
H,0,-0.0888134743,0.4769911261,-0.9712282656
H,0,-0.4109668973,2.1699641497,-1.3041773708
H,0,2.0236412076,2.6919402604,-0.8417459667
H,0,1.8337329837,1.5433112338,-2.1594531273
C,0,4.0617581865,0.8111041773,-0.6480122611
H,0,3.4087126385,1.7748929424,1.6551901935
H,0,2.1625291034,3.2377236083,1.6452510435
H,0,2.5308341374,2.0562777804,3.3358399814
H,0,0.6830924567,0.6487168621,2.5846920215
H,0,4.2450215719,0.6744127006,-1.7170785276
H,0,4.4209541197,1.8046942862,-0.367778617

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203491	E(Thermal)=	0.211698
E(SCF)=	-298.516874	DE(MP2)=	-1.316609
DE(CBS)=	-0.124050	DE(MP34)=	-0.089980
DE(CCSD)=	-0.041516	DE(Int)=	0.044685
DE(Empirical)=	-0.066748		
CBS-QB3 (0 K)=	-299.907600	CBS-QB3 Energy=	-299.899393
CBS-QB3 Enthalpy=	-299.898449	CBS-QB3 Free Energy=	-299.939453

4e-11

B3LYP/6-31+G**
E(RB+HF-LYP) = -300.612968263

Zero-point correction= 0.206108 (Hartree/Particle)
Thermal correction to Energy= 0.214260
Thermal correction to Enthalpy= 0.215204
Thermal correction to Gibbs Free Energy= 0.174230
Sum of electronic and ZPE= -300.406860
Sum of electronic and thermal Energies= -300.398709
Sum of electronic and thermal Enthalpies= -300.397765
Sum of electronic and thermal Free Energies= -300.438738

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.450	33.122	86.236

C,0,-0.0871527454,0.345630977,-0.1869105405
C,0,0.0237357061,0.1031985126,1.3193800628
C,0,1.2744783752,0.1507503621,1.9972893795
B,0,0.3740562622,1.5589671347,2.4064098856
H,0,-0.7654193349,-0.4964103982,1.765232463
C,0,2.6000281795,0.339838914,1.2524419676
H,0,1.3528946449,-0.4680132583,2.8879281886
H,0,0.1034056634,1.5074201876,3.5714130694
H,0,-0.7386451931,1.4824667187,1.8596021392
H,0,0.8858585938,2.506810331,1.8817943945
H,0,3.2003585685,1.0746599186,1.8033871084
C,0,3.3928027181,-0.9825113601,1.2517389788
H,0,-0.8485655499,-0.3331405995,-0.5879161144
H,0,-0.4471030902,1.3617813249,-0.3782585399
C,0,1.2558393516,0.1403036651,-0.9071688569
H,0,1.1698689753,0.494575889,-1.9408880116
C,0,2.3832121756,0.8813053193,-0.1770777166
H,0,1.4862300543,-0.9310983003,-0.964133844
H,0,3.3211872381,0.8010630258,-0.7395889484
H,0,2.1351310174,1.9487929118,-0.1290758741
H,0,4.3747968679,-0.8459780628,0.7845422099
H,0,3.557952351,-1.3410722617,2.2740075197
H,0,2.8669811705,-1.7750539511,0.7069610793

B3LYP/6-31G*
E(RB+HF-LYP) = -300.585116455

Zero-point correction= 0.207555 (Hartree/Particle)

Thermal correction to Energy= 0.215636
Thermal correction to Enthalpy= 0.216580
Thermal correction to Gibbs Free Energy= 0.175728
Sum of electronic and ZPE= -300.377562
Sum of electronic and thermal Energies= -300.369480
Sum of electronic and thermal Enthalpies= -300.368536
Sum of electronic and thermal Free Energies= -300.409388

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.314	32.751	85.981

C,0,-0.0850636028,0.3465259107,-0.1851420279
C,0,0.0252791682,0.1035992228,1.321847572
C,0,1.2770747033,0.1592343926,2.0023595696
B,0,0.3802403791,1.5600216285,2.4045438855
H,0,-0.7580949344,-0.5075183866,1.7638588724
C,0,2.6016902819,0.3415716015,1.2541972249
H,0,1.3566058347,-0.4666309545,2.8886153109
H,0,0.1031043291,1.5164073564,3.5690366002
H,0,-0.7382457064,1.4631089775,1.859248481
H,0,0.8700998112,2.5135720946,1.8678350549
H,0,3.2083510238,1.0730214625,1.8033944514
C,0,3.3867994328,-0.9843573445,1.2494232448
H,0,-0.8473409742,-0.3303954917,-0.5887779976
H,0,-0.4430318328,1.3637913613,-0.3757434165
C,0,1.2581467073,0.1411419767,-0.903904374
H,0,1.1720393702,0.4935904113,-1.9387464473
C,0,2.3838030658,0.8839964289,-0.1741046737
H,0,1.4895921456,-0.9305190526,-0.9592191807
H,0,3.321704696,0.8064264667,-0.738114067
H,0,2.1329340932,1.951184107,-0.1248256342
H,0,4.3686408703,-0.8537260558,0.778968313
H,0,3.5527201106,-1.3458482264,2.2712131748
H,0,2.8548830275,-1.7739098866,0.7051430636

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199253	E(Thermal)=	0.207648
E(QCISD(T))=	-299.564976	E(Empiric)=	-0.155480
DE(Plus)=	-0.014447	DE(2DF)=	-0.301158
E(Delta-G3)=	-0.435431	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.272239	G3 Energy=	-300.263844
G3 Enthalpy=	-300.262900	G3 Free Energy=	-300.304287

CBS-QB3

C,0,-0.083868851,0.3427904721,-0.1841847099
C,0,0.026885378,0.1038801721,1.3204997165
C,0,1.2754335114,0.1531950796,1.9975572645
B,0,0.3764015454,1.5603766134,2.403489375
H,0,-0.7593942598,-0.4949687818,1.7660763487
C,0,2.5992758823,0.3393826669,1.2528163542
H,0,1.3536878702,-0.4630942968,2.8868621901
H,0,0.1049259317,1.5112554041,3.5647551653
H,0,-0.7369570098,1.4770441493,1.8566704199
H,0,0.8804655851,2.5060459834,1.8759792803
H,0,3.1999666467,1.0706304866,1.80343207
C,0,3.387520525,-0.9836013971,1.2487447553
H,0,-0.8410804913,-0.3379933966,-0.5839650556
H,0,-0.4476001591,1.3551205691,-0.3755763141
C,0,1.2579508143,0.1421447662,-0.904386583
H,0,1.171303031,0.4978472027,-1.9351849152
C,0,2.3830414811,0.8827815587,-0.1740077517
H,0,1.4900705671,-0.926560729,-0.9642740999
H,0,3.3194297928,0.8045960409,-0.7350438053
H,0,2.134750649,1.9478749732,-0.1237958591
H,0,4.3668708865,-0.8493707063,0.780122488
H,0,3.5538615196,-1.3422081897,2.2686084089

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203510	E(Thermal)=	0.211743
E(SCF)=	-298.514394	DE(MP2)=	-1.317677
DE(CBS)=	-0.124114	DE(MP34)=	-0.089776
DE(CCSD)=	-0.041530	DE(Int)=	0.044693
DE(Empirical)=	-0.066741		
CBS-QB3 (0 K)=	-299.906030	CBS-QB3 Energy=	-299.897797
CBS-QB3 Enthalpy=	-299.896853	CBS-QB3 Free Energy=	-299.937960

4e-12

B3LYP/6-31+G**
E(RB+HF-LYP) = -300.612404670

Zero-point correction= 0.206286 (Hartree/Particle)
Thermal correction to Energy= 0.214471
Thermal correction to Enthalpy= 0.215415
Thermal correction to Gibbs Free Energy= 0.174296

Sum of electronic and ZPE= -300.406119
Sum of electronic and thermal Energies= -300.397934
Sum of electronic and thermal Enthalpies= -300.396989
Sum of electronic and thermal Free Energies= -300.438109

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.583	33.135	86.543

C,0,2.1886119618,0.6255082353,1.2738175288
H,0,2.635197852,-0.1605203298,1.8791856744
C,0,0.9786850166,1.204500577,1.7421008773
C,0,-0.0367685949,1.8378852735,0.7820998421
C,0,0.2493934982,1.5308701912,-0.6997623441
C,0,1.7491335077,1.609752315,-1.0187538916
C,0,2.5637045819,0.583379021,-0.2044439609
C,0,2.3766168382,-0.8617276625,-0.7130026787
B,0,2.3143487852,2.1964225325,2.2377727932
H,0,-0.0683930132,2.9216420366,0.9340148598
H,0,-1.0339386449,1.4635099756,1.0426013699
H,0,-0.122710681,0.5283391004,-0.9469206709
H,0,-0.3069656572,2.2288276396,-1.3359598966
H,0,2.1169623978,2.6188207483,-0.7980683974
H,0,1.924227623,1.4360568173,-2.0874588947
H,0,3.6288151886,0.8245649014,-0.3059244396
H,0,3.0078451233,-1.5618786871,-0.1545965
H,0,2.6592688485,-0.9279150435,-1.769032225
H,0,1.3402855575,-1.2016102058,-0.6199030565
H,0,3.3576997965,1.7033602524,1.7782652084
H,0,2.2138731304,3.2459953892,1.6732498851
H,0,2.45185304,2.1032793085,3.4232189757
H,0,0.5544928438,0.7660596137,2.6402059413

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199417	E(Thermal)=	0.207848
E(QCISD(T))=	-299.564356	E(Empiric)=	-0.155480
DE(Plus)=	-0.014242	DE(2DF)=	-0.301370
E(Delta-G3)=	-0.435482	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.271513	G3 Energy=	-300.263081
G3 Enthalpy=	-300.262137	G3 Free Energy=	-300.303681

CBS-QB3
C,0,2.1908112516,0.627874039,1.2737185408

H,0,2.6376057124,-0.154798196,1.8788491601
C,0,0.9810015435,1.2027517991,1.7405975701
C,0,-0.0351420778,1.831829418,0.781489624
C,0,0.2536110678,1.5312936402,-0.6995799194
C,0,1.7522172346,1.6106956465,-1.0159187783
C,0,2.5635182106,0.5835297188,-0.2028051177
C,0,2.3706392774,-0.859217378,-0.7107752282
B,0,2.3108322385,2.1988081659,2.2344200896
H,0,-0.0727547345,2.912586061,0.9368983463
H,0,-1.0287515559,1.4521777805,1.038955587
H,0,-0.1179942248,0.5320576281,-0.9512693555
H,0,-0.3002724808,2.2306732909,-1.3324389709
H,0,2.1199035023,2.6170953678,-0.7935323244
H,0,1.9283814001,1.4391170571,-2.0825017912
H,0,3.626903009,0.8214447696,-0.3044529119
H,0,3.0017648387,-1.5594099605,-0.1562918008
H,0,2.6475577795,-0.925686715,-1.766191344
H,0,1.3358248517,-1.1957476902,-0.6123944551
H,0,3.354399742,1.7028551442,1.7751161109
H,0,2.213405288,3.2435602001,1.6683793791
H,0,2.4502226574,2.1075512156,3.4161696434

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203669	E(Thermal)=	0.211941
E(SCF)=	-298.514344	DE(MP2)=	-1.317115
DE(CBS)=	-0.123991	DE(MP34)=	-0.089915
DE(CCSD)=	-0.041462	DE(Int)=	0.044667
DE(Empirical)=	-0.066756		
CBS-QB3 (0 K)=	-299.905247	CBS-QB3 Energy=	-299.896976
CBS-QB3 Enthalpy=	-299.896032	CBS-QB3 Free Energy=	-299.937300

4e-13
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.611797514

Zero-point correction= 0.206152 (Hartree/Particle)
Thermal correction to Energy= 0.214284
Thermal correction to Enthalpy= 0.215228
Thermal correction to Gibbs Free Energy= 0.174180
Sum of electronic and ZPE= -300.405645
Sum of electronic and thermal Energies= -300.397513
Sum of electronic and thermal Enthalpies= -300.396569
Sum of electronic and thermal Free Energies= -300.437617

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.465	33.150	86.393

C,0,2.2011568048,0.5656527177,1.2342258802
H,0,2.5698180734,-0.2254961217,1.8826019292
C,0,1.065975557,1.3029669161,1.6542930143
C,0,0.0615134267,1.9154201386,0.6601699311
C,0,0.4170574284,1.6082652956,-0.8182042723
C,0,1.9267881753,1.5413362738,-1.0864292268
C,0,2.5618183954,0.4364776643,-0.2334081454
H,0,2.1743669126,-0.5407916174,-0.5585828949
B,0,2.5142675448,2.1806177065,2.0801261182
C,0,-0.2096404758,3.409878337,0.8980188617
H,0,-0.8842022546,1.396482066,0.8710003753
H,0,-0.0189937014,0.6390529219,-1.0982207071
H,0,-0.0524071145,2.3559896715,-1.4683475243
H,0,2.4016056687,2.502619971,-0.8609752708
H,0,2.1127361407,1.3362421569,-2.1469444542
H,0,3.6487220923,0.401171754,-0.3637372504
H,0,3.50200281,1.550735467,1.6790879217
H,0,2.5508728363,3.1888052239,1.4410636567
H,0,2.6173453436,2.1684469254,3.2725705542
H,0,0.6174084872,0.9950796511,2.5946071953
H,0,-0.4129067103,3.6113226428,1.9554240664
H,0,0.6466126496,4.0248795143,0.6064193496
H,0,-1.0803830901,3.7343897238,0.3163888925

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199391	E(Thermal)=	0.208709
E(QCISD(T))=	-299.568325	E(Empiric)=	-0.155480
DE(Plus)=	-0.014041	DE(2DF)=	-0.300446
E(Delta-G3)=	-0.436358	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.275258	G3 Energy=	-300.265940
G3 Enthalpy=	-300.264996	G3 Free Energy=	-300.308286

CBS-QB3

C,0,2.2007626961,0.5681350648,1.2332528348
H,0,2.5670955232,-0.2227593465,1.8791030532
C,0,1.0664838776,1.3028909801,1.6532469433
C,0,0.0625584862,1.9146043315,0.660666787
C,0,0.4164648373,1.6069564696,-0.8161229521
C,0,1.9244337899,1.5427536257,-1.0847467856

C,0,2.560823778,0.4406056266,-0.2322842647
H,0,2.1769107776,-0.5357822697,-0.5579048285
B,0,2.5105725475,2.1821870936,2.0781398791
C,0,-0.2055293038,3.4078358443,0.8975554323
H,0,-0.8815924228,1.397422261,0.8710553782
H,0,-0.0175845636,0.638577616,-1.0935923514
H,0,-0.0542989518,2.3515602213,-1.4649466255
H,0,2.3967803166,2.5031404998,-0.8606539509
H,0,2.1100015761,1.337956903,-2.1431088901
H,0,3.6455917837,0.4076147288,-0.3621213255
H,0,3.4973462536,1.5445231996,1.6840641072
H,0,2.5558430169,3.1838256783,1.4361760537
H,0,2.6125014999,2.1729723054,3.2670845246
H,0,0.6183875715,0.9921998602,2.5900000256
H,0,-0.4128892289,3.6089057087,1.952177852
H,0,0.6523224162,4.0191528493,0.6106526638

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203543	E(Thermal)=	0.211762
E(SCF)=	-298.513321	DE(MP2)=	-1.317808
DE(CBS)=	-0.124072	DE(MP34)=	-0.089799
DE(CCSD)=	-0.041546	DE(Int)=	0.044696
DE(Empirical)=	-0.066730		
CBS-QB3 (0 K)=	-299.905039	CBS-QB3 Energy=	-299.896819
CBS-QB3 Enthalpy=	-299.895875	CBS-QB3 Free Energy=	-299.937077

4e-14
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.612065397

Zero-point correction= 0.206233 (Hartree/Particle)
Thermal correction to Energy= 0.214284
Thermal correction to Enthalpy= 0.215228
Thermal correction to Gibbs Free Energy= 0.174391
Sum of electronic and ZPE= -300.405832
Sum of electronic and thermal Energies= -300.397781
Sum of electronic and thermal Enthalpies= -300.396837
Sum of electronic and thermal Free Energies= -300.437675

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.465	32.980	85.950

C,0,-0.0112661662,0.0526971792,-0.01280303
C,0,0.1215195957,0.11910284,1.5138597928
C,0,1.5612979892,0.3395325737,1.9639056857
C,0,2.5272815507,0.8761066747,1.0705018198
C,0,2.1989092342,1.3236250967,-0.3617583524
C,0,0.6784902882,1.2626196653,-0.654699298
H,0,2.4923313694,2.3830956231,-0.3738227055
B,0,2.6804264879,-0.9072780526,1.5607938989
H,0,3.3856284756,1.3774358432,1.5117251248
H,0,1.6853240223,0.5777068095,3.0167127619
H,0,3.3586551918,-1.1436001623,2.5190518817
H,0,3.4877597432,-0.4690801221,0.7277394791
H,0,2.0875852305,-1.7522226878,0.9548647212
H,0,-0.2774956572,-0.7902641153,1.9766818957
H,0,-0.4897590343,0.9547781918,1.8866674417
C,0,3.03598753,0.6257639303,-1.4465067026
H,0,0.5231377876,1.2683979767,-1.7400933777
H,0,0.2035954243,2.1748634728,-0.268664784
H,0,-1.0709392973,0.0328921548,-0.2928069244
H,0,0.4306385869,-0.8786559962,-0.3866640231
H,0,2.8674761256,1.1042391197,-2.417160656
H,0,4.1072144274,0.6823842573,-1.2245552621
H,0,2.7683600948,-0.4319812724,-1.5341563874

B3LYP/6-31G*
E(RB+HF-LYP) = -300.584357690

Zero-point correction= 0.207670 (Hartree/Particle)
Thermal correction to Energy= 0.215657
Thermal correction to Enthalpy= 0.216601
Thermal correction to Gibbs Free Energy= 0.175871
Sum of electronic and ZPE= -300.376687
Sum of electronic and thermal Energies= -300.368701
Sum of electronic and thermal Enthalpies= -300.367757
Sum of electronic and thermal Free Energies= -300.408486

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.327	32.614	85.723

C,0,-0.0090903782,0.0543652561,-0.0136845402
C,0,0.1224962027,0.1174353168,1.5126898846
C,0,1.5625250564,0.3317980574,1.964272846

C,0,2.5288461481,0.8764342415,1.071790509
C,0,2.2004541968,1.3244449769,-0.3610268794
C,0,0.6797698182,1.266190737,-0.6515537806
H,0,2.4971791367,2.3831960885,-0.3789260205
B,0,2.67509565,-0.9069055843,1.5605710111
H,0,3.3798279731,1.3878553084,1.5169730904
H,0,1.6818100272,0.5793303652,3.0160227214
H,0,3.3585949237,-1.149497131,2.5142593585
H,0,3.4891077852,-0.4465180885,0.7368419502
H,0,2.100999158,-1.7495791254,0.9322036351
H,0,-0.280374104,-0.7921922271,1.9727517871
H,0,-0.4888541055,0.9534819063,1.8861338732
C,0,3.031886344,0.6175054453,-1.4433400456
H,0,0.5223395389,1.2771861233,-1.7370993941
H,0,0.2062209839,2.1775548304,-0.2608596653
H,0,-1.0689372079,0.0342004401,-0.2949567646
H,0,0.4345231488,-0.8758626438,-0.3893454149
H,0,2.8575432102,1.0857270773,-2.4186275525
H,0,4.1047715179,0.677906372,-1.2277177645
H,0,2.7654229759,-0.4418977423,-1.5185588445

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199364	E(Thermal)=	0.207665
E(QCISD(T))=	-299.564244	E(Empiric)=	-0.155480
DE(Plus)=	-0.014084	DE(2DF)=	-0.301249
E(Delta-G3)=	-0.435830	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.271523	G3 Energy=	-300.263221
G3 Enthalpy=	-300.262277	G3 Free Energy=	-300.303539

CBS-QB3

C,0,-0.0091582976,0.0530901185,-0.0117648478
C,0,0.1234418123,0.12095364,1.5130130404
C,0,1.5617157585,0.3393808638,1.9620711791
C,0,2.5265271752,0.8740241574,1.0697673201
C,0,2.1984208689,1.3222227648,-0.3602011618
C,0,0.6797936151,1.2611054629,-0.6538874167
H,0,2.4897836486,2.3800381374,-0.3719569145
B,0,2.6768258999,-0.9078154045,1.5588100298
H,0,3.382132599,1.3748146488,1.5107202986
H,0,1.6860393785,0.5778224156,3.0121791705
H,0,3.3539007947,-1.1452620895,2.5130824466
H,0,3.4855198098,-0.4643635901,0.7284115115
H,0,2.0889975827,-1.7480667666,0.9488360864
H,0,-0.2754337446,-0.785858976,1.9757561922

H,0,-0.4863648166,0.955490725,1.8848405917
C,0,3.0347095889,0.6254679423,-1.4435729898
H,0,0.5255680606,1.2657906218,-1.7371185307
H,0,0.2058071403,2.1721193319,-0.2700290745
H,0,-1.0666141192,0.0327915071,-0.2913467827
H,0,0.4319704451,-0.8769387978,-0.3836204837
H,0,2.8627786898,1.099846506,-2.4134209084
H,0,4.1042785706,0.6871289901,-1.2247105945

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203641	E(Thermal)=	0.211778
E(SCF)=	-298.513209	DE(MP2)=	-1.318143
DE(CBS)=	-0.124175	DE(MP34)=	-0.089803
DE(CCSD)=	-0.041567	DE(Int)=	0.044703
DE(Empirical)=	-0.066732		
CBS-QB3 (0 K)=	-299.905285	CBS-QB3 Energy=	-299.897148
CBS-QB3 Enthalpy=	-299.896204	CBS-QB3 Free Energy=	-299.937187

4e-15
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.648634795

Zero-point correction= 0.207314 (Hartree/Particle)
Thermal correction to Energy= 0.216107
Thermal correction to Enthalpy= 0.217051
Thermal correction to Gibbs Free Energy= 0.174799
Sum of electronic and ZPE= -300.441320
Sum of electronic and thermal Energies= -300.432528
Sum of electronic and thermal Enthalpies= -300.431584
Sum of electronic and thermal Free Energies= -300.473836

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.609	34.886	88.927

C,0,2.3761957548,0.8439278374,-0.1678261163
C,0,2.5457511215,0.4536613886,1.3092944122
C,0,1.1866727529,0.4961786158,2.039965413
C,0,0.1628356175,-0.4248880421,1.3421439798
C,0,-0.0263836177,-0.0392895471,-0.1381767583
C,0,1.3299366604,-0.0370033943,-0.8687853526
C,0,-1.0456097697,-0.94792435,-0.8355107664

B,0,0.6725463121,1.9030653268,2.4707668727
H,0,0.5037253289,-1.4710115981,1.3884531111
H,0,1.3416248933,0.1074629025,3.0764808996
H,0,-0.4871137048,2.0806869501,2.716166858
H,0,-0.8024630903,-0.3835551106,1.8620704254
H,0,1.4404360633,2.801050271,2.6717742939
H,0,3.2635584776,1.1230927932,1.7978051208
H,0,2.9679091188,-0.5610318467,1.361862835
H,0,-0.4202292463,0.9909383318,-0.1619438313
H,0,1.1927262923,0.2912111909,-1.9074656853
H,0,1.7046623154,-1.0712754409,-0.9168278164
H,0,3.3372345848,0.7751650585,-0.6924807507
H,0,2.0642220631,1.897785379,-0.2271921917
H,0,-1.1964941973,-0.6500636603,-1.8796359347
H,0,-0.7064210266,-1.9916335865,-0.8331256972
H,0,-2.018976704,-0.9134574693,-0.3326173205

G3B3
E(RB+HF-LYP) = -300.621276047

Zero-point correction= 0.208778 (Hartree/Particle)
Thermal correction to Energy= 0.217549
Thermal correction to Enthalpy= 0.218493
Thermal correction to Gibbs Free Energy= 0.176253
Sum of electronic and ZPE= -300.412498
Sum of electronic and thermal Energies= -300.403727
Sum of electronic and thermal Enthalpies= -300.402783
Sum of electronic and thermal Free Energies= -300.445023

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.514	34.611	88.902

C,0,2.3750804884,0.8447040568,-0.1646820332
C,0,2.5459681455,0.4507182662,1.3105008546
C,0,1.1883617182,0.4917571862,2.0433520983
C,0,0.1647539958,-0.4280494861,1.3435314397
C,0,-0.0256505736,-0.0381386682,-0.1349710835
C,0,1.329686061,-0.0356926452,-0.8664919523
C,0,-1.0452752398,-0.9442987526,-0.8334447747
B,0,0.6703215244,1.9033459399,2.4606274812
H,0,0.5060735079,-1.4744365142,1.3878823504
H,0,1.3453830289,0.0979528877,3.0768542908
H,0,-0.4906321249,2.0814203309,2.7043215951

H,0,-0.8005117464,-0.3888022206,1.8646624856
H,0,1.43496673,2.8076944398,2.65116791
H,0,3.2650978945,1.1188636315,1.799881299
H,0,2.9682073358,-0.5644534885,1.3604608187
H,0,-0.4182108677,0.9930796823,-0.1553409332
H,0,1.192668169,0.2929824066,-1.9055373632
H,0,1.7050828135,-1.0699406336,-0.9154432431
H,0,3.3363423561,0.7793560244,-0.6903423169
H,0,2.0612674344,1.898640432,-0.2207688567
H,0,-1.1966776891,-0.6440821576,-1.8773905649
H,0,-0.7071278583,-1.9888001012,-0.8339520471
H,0,-2.0188291036,-0.9107286164,-0.3296814546

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200427	E(Thermal)=	0.209519
E(QCISD(T))=	-299.601188	E(Empiric)=	-0.155480
DE(Plus)=	-0.013970	DE(2DF)=	-0.299921
E(Delta-G3)=	-0.435652	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.305784	G3 Energy=	-300.296692
G3 Enthalpy=	-300.295748	G3 Free Energy=	-300.338558

CBS-QB3

C,0,2.3759566978,0.8419606806,-0.1659479864
C,0,2.5427559384,0.4540812548,1.3102316738
C,0,1.1838516568,0.4970480803,2.0383108748
C,0,0.161195771,-0.4225292883,1.3401774674
C,0,-0.0245769203,-0.0380606567,-0.1391585479
C,0,1.3314296915,-0.037964593,-0.866953222
C,0,-1.0419616552,-0.9458032919,-0.8363875566
B,0,0.6711448767,1.8999675959,2.4710801991
H,0,0.4999885771,-1.4669483144,1.3889183384
H,0,1.3392976615,0.1047432635,3.0718297734
H,0,-0.4857608064,2.0763274733,2.7164817747
H,0,-0.8029599951,-0.3790776146,1.8574388581
H,0,1.4369427772,2.7965776649,2.6695933618
H,0,3.2574182184,1.1231420815,1.7987474564
H,0,2.96417563,-0.5583886294,1.3657622139
H,0,-0.41629425,0.9906298998,-0.1644828111
H,0,1.1962574423,0.2892301086,-1.9038359432
H,0,1.7044176876,-1.0706270106,-0.9138617308
H,0,3.3359835227,0.7716985364,-0.6875489166
H,0,2.0660985598,1.8941563011,-0.2277311541
H,0,-1.1905076801,-0.6494867758,-1.8791460532
H,0,-0.7040820569,-1.9877906796,-0.8320156708

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.204760	E(Thermal)=	0.213633
E(SCF)=	-298.573623	DE(MP2)=	-1.291549
DE(CBS)=	-0.122153	DE(MP34)=	-0.095906
DE(CCSD)=	-0.038168	DE(Int)=	0.044243
DE(Empirical)=	-0.067223		
CBS-QB3 (0 K)=	-299.939618	CBS-QB3 Energy=	-299.930746
CBS-QB3 Enthalpy=	-299.929802	CBS-QB3 Free Energy=	-299.972192

4e-16
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.646391411

Zero-point correction= 0.207430 (Hartree/Particle)
Thermal correction to Energy= 0.216208
Thermal correction to Enthalpy= 0.217153
Thermal correction to Gibbs Free Energy= 0.174978
Sum of electronic and ZPE= -300.438962
Sum of electronic and thermal Energies= -300.430183
Sum of electronic and thermal Enthalpies= -300.429239
Sum of electronic and thermal Free Energies= -300.471413

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.673	34.885	88.764

C,0,2.3309685109,0.895654131,-0.1594097789
C,0,2.460059115,0.3899554838,1.2913993172
C,0,1.0811979464,0.4950197752,1.9969503357
C,0,0.0298383591,-0.3435176358,1.2333732646
C,0,-0.1053841312,0.1507214224,-0.2164095577
C,0,1.2481286264,0.136925286,-0.9440333995
B,0,0.5791984144,1.8961563575,2.4687661318
C,0,3.604324253,1.0839875732,2.039325448
H,0,0.3309289996,-1.4016352954,1.2222148767
H,0,1.1910412447,0.0497684892,3.0161653916
H,0,-0.5841846938,2.0476635678,2.7150399399
H,0,-0.9399806171,-0.2936841086,1.7420517263
H,0,1.318199574,2.8086310165,2.6963514875
H,0,2.7110591474,-0.6820279587,1.2358587903
H,0,-0.8333814937,-0.4624776379,-0.7620311184

H,0,-0.5060116625,1.1762191936,-0.2089112655
H,0,1.1434829134,0.5601352905,-1.9508842626
H,0,1.5707044995,-0.9061353981,-1.0770347025
H,0,3.2972107734,0.8068274992,-0.6732395494
H,0,2.0881315744,1.9699302106,-0.1389574036
H,0,4.5641080837,0.8721182765,1.5540791113
H,0,3.4758748654,2.1708296442,2.0620014483
H,0,3.6727786977,0.7355498174,3.0771167692

B3LYP/6-31G*
E(RB+HF-LYP) = -300.619245873

Zero-point correction= 0.208897 (Hartree/Particle)
Thermal correction to Energy= 0.217651
Thermal correction to Enthalpy= 0.218596
Thermal correction to Gibbs Free Energy= 0.176428
Sum of electronic and ZPE= -300.410348
Sum of electronic and thermal Energies= -300.401593
Sum of electronic and thermal Enthalpies= -300.400649
Sum of electronic and thermal Free Energies= -300.442817

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.575	34.603	88.771

C,0,2.3299792102,0.8965767895,-0.1574991791
C,0,2.4604663223,0.3883443656,1.2917765555
C,0,1.0833156989,0.4924244669,1.9998128071
C,0,0.0315235015,-0.3449461966,1.2356650894
C,0,-0.1045871248,0.1511649881,-0.212608868
C,0,1.2478597955,0.1366526316,-0.9409295465
B,0,0.5789805332,1.8987187343,2.4589445441
C,0,3.603574525,1.0826302381,2.0399762893
H,0,0.3323928327,-1.4034483514,1.2235393026
H,0,1.1940811914,0.0432871642,3.0165736332
H,0,-0.5839123045,2.04892307,2.7128541985
H,0,-0.9386833821,-0.2959936632,1.7447453185
H,0,1.3148680661,2.8196735866,2.6681636299
H,0,2.7123009383,-0.6836754531,1.234345409
H,0,-0.8345792538,-0.4600871124,-0.7586325605
H,0,-0.5036721864,1.1777577317,-0.2031477306
H,0,1.142562681,0.5580761749,-1.9489667535
H,0,1.5706350666,-0.9068558626,-1.0724019291
H,0,3.2961315015,0.8107891377,-0.6729343833

H,0,2.0848014732,1.9706560544,-0.1359113754
H,0,4.5634854737,0.8796104999,1.5499793073
H,0,3.469431987,2.1690671813,2.0708076526
H,0,3.6773364534,0.7272688247,3.075631589

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200532	E(Thermal)=	0.209612
E(QCISD(T))=	-299.599523	E(Empiric)=	-0.155480
DE(Plus)=	-0.013677	DE(2DF)=	-0.300201
E(Delta-G3)=	-0.435859	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.304207	G3 Energy=	-300.295127
G3 Enthalpy=	-300.294183	G3 Free Energy=	-300.336931

CBS-QB3

C,0,2.3344411355,0.8938545639,-0.1557425501
C,0,2.4572170299,0.3844443928,1.2926044918
C,0,1.0783594546,0.4943825003,1.9946095235
C,0,0.0249514394,-0.3347981667,1.2265229118
C,0,-0.1031721392,0.1632273813,-0.2206898574
C,0,1.2506722525,0.1437602651,-0.9439016404
B,0,0.5849240943,1.8931782849,2.4709796073
C,0,3.6009467258,1.0708323863,2.0444796245
H,0,0.3190952672,-1.3925495146,1.2149138639
H,0,1.1838490072,0.0416972567,3.0092395997
H,0,-0.575317184,2.0488118857,2.7157167477
H,0,-0.9436219189,-0.2795961141,1.7321066026
H,0,1.3266033768,2.7993640624,2.6998650091
H,0,2.7017552221,-0.6866107062,1.2355768456
H,0,-0.8314177662,-0.4435457778,-0.7685998768
H,0,-0.4978585142,1.1888269813,-0.2122990437
H,0,1.1508709712,0.5694299712,-1.9477744628
H,0,1.5671807092,-0.8986181242,-1.0791047666
H,0,3.2994452204,0.8007059419,-0.6662429813
H,0,2.0982953704,1.9674631895,-0.1337468541
H,0,4.5591381081,0.8585150038,1.5607917333
H,0,3.4754594637,2.1558661733,2.0716867312

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.204888	E(Thermal)=	0.213747
E(SCF)=	-298.570965	DE(MP2)=	-1.292743
DE(CBS)=	-0.122181	DE(MP34)=	-0.095793
DE(CCSD)=	-0.038253	DE(Int)=	0.044244
DE(Empirical)=	-0.067211		

CBS-QB3 (0 K)= -299.938015 CBS-QB3 Energy= -299.929155
CBS-QB3 Enthalpy= -299.928211 CBS-QB3 Free Energy= -299.970524

4e-17
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.648533503

Zero-point correction= 0.207547 (Hartree/Particle)
Thermal correction to Energy= 0.216613
Thermal correction to Enthalpy= 0.217557
Thermal correction to Gibbs Free Energy= 0.174518
Sum of electronic and ZPE= -300.440986
Sum of electronic and thermal Energies= -300.431921
Sum of electronic and thermal Enthalpies= -300.430977
Sum of electronic and thermal Free Energies= -300.474015

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.927	35.103	90.583

C,0,2.6654967145,1.2740502262,1.0641212628
H,0,3.3424699082,0.6932125278,1.7036040909
C,0,1.2322722818,1.3229947764,1.6919443804
C,0,0.2646905422,2.0665475637,0.7489021256
C,0,0.2565493624,1.4699937019,-0.6663706911
C,0,1.6704442284,1.4211907581,-1.263523535
C,0,2.6606485664,0.6694804341,-0.3565081952
H,0,2.3081474521,-0.3701156272,-0.2665892733
B,0,1.435229462,1.9510174144,3.1084913206
H,0,0.5604431765,3.1246953999,0.6964474084
H,0,-0.7504747479,2.0526803248,1.165953772
H,0,-0.155817449,0.4509409353,-0.6283530364
H,0,-0.4083623062,2.0498155357,-1.3188974687
H,0,2.0374287536,2.4483119571,-1.4137827163
H,0,1.6492897543,0.9512982041,-2.2556452471
C,0,4.073483998,0.6439406707,-0.952717521
H,0,3.0823598774,2.2917175906,1.0062544217
H,0,1.2402141452,3.1180734232,3.3039824488
H,0,1.864905067,1.2898352123,4.0106241965
H,0,0.9075437011,0.2738662709,1.7862742509
H,0,4.0743569284,0.1812993224,-1.9465763054
H,0,4.4739473962,1.6600337907,-1.0587997949
H,0,4.7653401875,0.0774225868,-0.3187068943

B3LYP/6-31G*
E(RB+HF-LYP) = -300.621482670

Zero-point correction= 0.209129 (Hartree/Particle)
Thermal correction to Energy= 0.218110
Thermal correction to Enthalpy= 0.219055
Thermal correction to Gibbs Free Energy= 0.176279
Sum of electronic and ZPE= -300.412353
Sum of electronic and thermal Energies= -300.403372
Sum of electronic and thermal Enthalpies= -300.402428
Sum of electronic and thermal Free Energies= -300.445204

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.866	34.798	90.029

C,0,2.6622945998,1.2740544017,1.0650030894
H,0,3.3423978831,0.6959411514,1.7045783416
C,0,1.2278226764,1.3165476112,1.6917777597
C,0,0.2620361231,2.0631102569,0.7493803006
C,0,0.2556053642,1.467713449,-0.6658394342
C,0,1.6694361136,1.4224880671,-1.2620002785
C,0,2.658646977,0.6696680037,-0.3553315337
H,0,2.3067072895,-0.3703912925,-0.2666822457
B,0,1.4435222709,1.9503886199,3.103652574
H,0,0.5587024774,3.1213181658,0.6987046329
H,0,-0.7541295255,2.0497622539,1.1650714826
H,0,-0.1549938487,0.4476326771,-0.6286107334
H,0,-0.4108942527,2.0466111741,-1.3183714483
H,0,2.0352269817,2.4507151195,-1.4093236813
H,0,1.6498769081,0.9555757547,-2.2560469333
C,0,4.0714357095,0.6469282093,-0.9501321863
H,0,3.0751197615,2.2935558318,1.0084860901
H,0,1.3088232276,3.1299416185,3.2786783496
H,0,1.8303384345,1.2836870284,4.022050211
H,0,0.9035961555,0.2672800455,1.7810798044
H,0,4.0736590912,0.1856262405,-1.9451878304
H,0,4.4713749559,1.6638315374,-1.0547498652
H,0,4.7640016264,0.0803170751,-0.3160574657

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200764	E(Thermal)=	0.210061
E(QCISD(T))=	-299.601213	E(Empiric)=	-0.155480

DE(Plus)=	-0.013863	DE(2DF)=	-0.299579
E(Delta-G3)=	-0.435490	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.304861	G3 Energy=	-300.295564
G3 Enthalpy=	-300.294619	G3 Free Energy=	-300.337969

CBS-QB3

C,0,2.6638881302,1.2724628803,1.0646817494
H,0,3.3368350208,0.6913849703,1.7043405759
C,0,1.2306284614,1.323686895,1.6902126682
C,0,0.2660893444,2.0674703184,0.7464364087
C,0,0.2595047636,1.4704490794,-0.6667442149
C,0,1.6724161753,1.4206549495,-1.261643966
C,0,2.6597559238,0.668623033,-0.3544659166
H,0,2.3072585997,-0.3685937904,-0.2652282175
B,0,1.4346452952,1.9523761249,3.1024671468
H,0,0.562637432,3.1231722197,0.6941194684
H,0,-0.7475189523,2.0551006471,1.1613529914
H,0,-0.1534774972,0.4539901019,-0.6289864353
H,0,-0.4026713628,2.0495988329,-1.3189556272
H,0,2.0398306794,2.4454163632,-1.4114098851
H,0,1.651860696,0.951644988,-2.2516960634
C,0,4.0716850759,0.6434008954,-0.9482647407
H,0,3.0817334537,2.2875250179,1.0088613137
H,0,1.2474172802,3.1183031956,3.2935453036
H,0,1.8563360107,1.2914600636,4.0046634038
H,0,0.905373427,0.2771765073,1.7852067783
H,0,4.073575052,0.1819649619,-1.9404148957
H,0,4.4715389803,1.6576814155,-1.0530637017

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.204997	E(Thermal)=	0.214134
E(SCF)=	-298.573748	DE(MP2)=	-1.290999
DE(CBS)=	-0.122147	DE(MP34)=	-0.095803
DE(CCSD)=	-0.038226	DE(Int)=	0.044234
DE(Empirical)=	-0.067243		
CBS-QB3 (0 K)=	-299.938934	CBS-QB3 Energy=	-299.929796
CBS-QB3 Enthalpy=	-299.928852	CBS-QB3 Free Energy=	-299.971991

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B3LYP/6-31+G**
E(RB+HF-LYP) = -300.648136900

Zero-point correction= 0.207764 (Hartree/Particle)
Thermal correction to Energy= 0.216681
Thermal correction to Enthalpy= 0.217625
Thermal correction to Gibbs Free Energy= 0.175123
Sum of electronic and ZPE= -300.440373
Sum of electronic and thermal Energies= -300.431456
Sum of electronic and thermal Enthalpies= -300.430512
Sum of electronic and thermal Free Energies= -300.473014

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.969	34.980	89.452

C,0,2.7115652179,1.2082289828,1.0043196362
H,0,3.4158742845,0.6430146278,1.6268619602
C,0,1.2912146554,1.227973075,1.6680605997
C,0,0.2641508784,1.9420279822,0.7595394119
C,0,0.2507984792,1.3370818817,-0.6566806725
C,0,1.6449367759,1.3221234619,-1.3008491335
C,0,2.6652977347,0.6025512848,-0.4095544919
H,0,2.3974557943,-0.4607517415,-0.3333785762
B,0,1.5513308869,1.8820964678,3.0633087389
H,0,0.5781769442,2.9946106957,0.6718234562
C,0,-1.1379411835,1.9202048721,1.3839966314
H,0,-0.1323178763,0.3064868889,-0.5983413402
H,0,-0.4525586782,1.8929147868,-1.2908057023
H,0,1.9781854724,2.3565510809,-1.4701667951
H,0,1.6016513603,0.8440668836,-2.2874210975
H,0,3.664722208,0.6461311622,-0.8608923099
H,0,3.103717754,2.2338177964,0.9349680707
H,0,1.4024140042,3.0607079156,3.2281357173
H,0,1.9987332864,1.2372117509,3.9682087788
H,0,0.9896368453,0.1734405083,1.779808001
H,0,-1.1456614425,2.4053335118,2.3677461135
H,0,-1.8662447776,2.4413979558,0.7518031675
H,0,-1.4908746241,0.8894041686,1.5171298357
Geom=AllCheck
E(RB+HF-LYP) = -300.621228830

Zero-point correction= 0.209241 (Hartree/Particle)
Thermal correction to Energy= 0.218165
Thermal correction to Enthalpy= 0.219110
Thermal correction to Gibbs Free Energy= 0.176544
Sum of electronic and ZPE= -300.411980

Sum of electronic and thermal Energies= -300.403056
Sum of electronic and thermal Enthalpies= -300.402112
Sum of electronic and thermal Free Energies= -300.444677

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.886	34.688	89.303

C,0,2.7111670521,1.2088232288,1.0036838354
H,0,3.4163158303,0.644349028,1.6267808056
C,0,1.2911872144,1.227048296,1.6672852299
C,0,0.2647569024,1.9422580081,0.7589631272
C,0,0.2506753188,1.3362443464,-0.6564178191
C,0,1.6445497939,1.3226021195,-1.300084941
C,0,2.6643956232,0.6028013075,-0.4092191792
H,0,2.3963284031,-0.4607582063,-0.3328270791
B,0,1.5498021881,1.8821492986,3.0627283518
H,0,0.5792982238,2.9947880074,0.6709997474
C,0,-1.1361998941,1.9200365019,1.3840943972
H,0,-0.131657897,0.3051162924,-0.5979928452
H,0,-0.4535786431,1.8909887637,-1.2912939647
H,0,1.9777516913,2.3575215142,-1.4683662096
H,0,1.6019863659,0.8453354062,-2.2875770009
H,0,3.6640963068,0.645434956,-0.8611343554
H,0,3.1031002019,2.2347815276,0.9350481907
H,0,1.4054686942,3.0623120032,3.2264600688
H,0,1.9930142,1.2370802398,3.9707461717
H,0,0.9898599277,0.1720907163,1.7768103303
H,0,-1.1423066696,2.4041589824,2.3691089899
H,0,-1.8653679921,2.4422801328,0.7528440434
H,0,-1.4903788418,0.8891835295,1.5169801051

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200899	E(Thermal)=	0.210090
E(QCISD(T))=	-299.601349	E(Empiric)=	-0.155480
DE(Plus)=	-0.013835	DE(2DF)=	-0.299933
E(Delta-G3)=	-0.435389	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.305087	G3 Energy=	-300.295896
G3 Enthalpy=	-300.294952	G3 Free Energy=	-300.337954

CBS-QB3

C,0,2.7092064649,1.2045188924,1.0063725485
H,0,3.4089122636,0.6391481905,1.6300085071
C,0,1.2888260152,1.2295181654,1.6679963611

C,0,0.2658021723,1.9443288684,0.7576840394
C,0,0.2527742737,1.3373547316,-0.6559560386
C,0,1.6462414972,1.3179753284,-1.2973325385
C,0,2.6625350048,0.5976860027,-0.4049494325
H,0,2.3930618152,-0.462892696,-0.3279165046
B,0,1.5498835339,1.8848203268,3.058723509
H,0,0.5825479432,2.9936308134,0.6688461923
C,0,-1.1351862455,1.9260252421,1.3800404508
H,0,-0.1330095861,0.3101337185,-0.5967466935
H,0,-0.446363824,1.8934428798,-1.2906770356
H,0,1.9816856473,2.3492642795,-1.4676547217
H,0,1.6031385598,0.8396642463,-2.2813068624
H,0,3.66044594,0.6382502418,-0.8545804651
H,0,3.1037811549,2.2269358367,0.9376870498
H,0,1.4038525541,3.0611197019,3.220451264
H,0,1.993518343,1.2409883226,3.9623599276
H,0,0.9853272695,0.1780747439,1.7815332163
H,0,-1.1428831618,2.4116406341,2.3613899435
H,0,-1.8604730156,2.4471085561,0.7478523908

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205192	E(Thermal)=	0.214187
E(SCF)=	-298.573156	DE(MP2)=	-1.292049
DE(CBS)=	-0.122148	DE(MP34)=	-0.095608
DE(CCSD)=	-0.038338	DE(Int)=	0.044228
DE(Empirical)=	-0.067230		
CBS-QB3 (0 K)=	-299.939109	CBS-QB3 Energy=	-299.930114
CBS-QB3 Enthalpy=	-299.929170	CBS-QB3 Free Energy=	-299.971808

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B3LYP/6-31+G**
E(RB+HF-LYP) = -300.644933269

Zero-point correction= 0.207897 (Hartree/Particle)
Thermal correction to Energy= 0.216871
Thermal correction to Enthalpy= 0.217815
Thermal correction to Gibbs Free Energy= 0.175021
Sum of electronic and ZPE= -300.437036
Sum of electronic and thermal Energies= -300.428062
Sum of electronic and thermal Enthalpies= -300.427118
Sum of electronic and thermal Free Energies= -300.469913

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.089	34.926	90.069

C,0,2.6576132225,1.1747397476,0.9974256687
H,0,3.3040987462,0.5503705788,1.6270641823
C,0,1.2338196372,1.3091834165,1.6379776631
C,0,0.3125965361,2.1262960644,0.7085296433
C,0,0.2503824194,1.5447335562,-0.7119846406
C,0,1.6546900837,1.4092305857,-1.3223497997
C,0,2.6210508459,0.5921903249,-0.4371402518
C,0,2.3072743734,-0.9128888205,-0.4510597622
B,0,1.4957757308,1.9095263519,3.0563980882
H,0,0.6831944907,3.1611783912,0.6617030626
H,0,-0.6971344329,2.1823938323,1.1350938594
H,0,-0.2433796845,0.5636265806,-0.683133337
H,0,-0.371786427,2.1812173979,-1.3537460531
H,0,2.0737393909,2.4162602352,-1.4626200304
H,0,1.5951096423,0.9573679163,-2.3211078906
H,0,3.6322454625,0.7112323024,-0.8523337538
H,0,3.0381965956,-1.4695864076,0.1468564761
H,0,2.3446297229,-1.3058133982,-1.4736616496
H,0,1.3140065033,-1.1387702678,-0.0498129464
H,0,3.1268767689,2.1684234829,0.9508065467
H,0,1.3715742261,3.0833491922,3.2689002759
H,0,1.9019661427,1.2136071428,3.9433120839
H,0,0.8356990029,0.2872537943,1.737590565

B3LYP/6-31G*
E(RB+HF-LYP) = -300.618060542

Zero-point correction= 0.209477 (Hartree/Particle)
Thermal correction to Energy= 0.218355
Thermal correction to Enthalpy= 0.219299
Thermal correction to Gibbs Free Energy= 0.176803
Sum of electronic and ZPE= -300.408584
Sum of electronic and thermal Energies= -300.399705
Sum of electronic and thermal Enthalpies= -300.398761
Sum of electronic and thermal Free Energies= -300.441257

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.020	34.609	89.441

C,0,2.6524709609,1.1754333155,1.0015124106
H,0,3.3003710983,0.5534921137,1.6330810869
C,0,1.2254054774,1.3036962723,1.6372483068
C,0,0.3082086236,2.1228498944,0.7057982255
C,0,0.2520237303,1.5424133595,-0.7148945114
C,0,1.6582291997,1.4103063931,-1.3200878962
C,0,2.6212187809,0.592852854,-0.4325821772
C,0,2.3066005088,-0.9111453142,-0.4474096031
B,0,1.4997870712,1.9105055995,3.0504353669
H,0,0.6789998288,3.1579845108,0.6616355583
H,0,-0.7037495572,2.1786894238,1.1282068022
H,0,-0.2398416011,0.5599014478,-0.6883514656
H,0,-0.3697808051,2.178140711,-1.3585589627
H,0,2.0766959404,2.4185010741,-1.4564696893
H,0,1.602865018,0.960730426,-2.3205813698
H,0,3.6341991001,0.7114250048,-0.8444962187
H,0,3.0367502367,-1.4691043412,0.1512483366
H,0,2.3438252046,-1.3040010315,-1.4705794018
H,0,1.3125023738,-1.136127904,-0.0461987964
H,0,3.1180522378,2.1712223864,0.9569809323
H,0,1.4412968996,3.0942666259,3.2390298899
H,0,1.8584099417,1.2115107502,3.9562959633
H,0,0.8276987307,0.2815784278,1.7314452129

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.201098	E(Thermal)=	0.210293
E(QCISD(T))=	-299.598298	E(Empiric)=	-0.155480
DE(Plus)=	-0.013560	DE(2DF)=	-0.299964
E(Delta-G3)=	-0.435815	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.302019	G3 Energy=	-300.292824
G3 Enthalpy=	-300.291880	G3 Free Energy=	-300.334946

CBS-QB3

C,0,2.6537065961,1.170728711,1.0032826131
H,0,3.2921107663,0.5446762656,1.6355640927
C,0,1.2272130198,1.310392119,1.6350636701
C,0,0.3146523078,2.12899446,0.7005977187
C,0,0.2591042512,1.5472964263,-0.7182453724
C,0,1.6648891281,1.4077831054,-1.3198633393
C,0,2.6223818038,0.5888875364,-0.4297059517
C,0,2.3029215261,-0.9130233942,-0.4440332043
B,0,1.487298257,1.9118199491,3.0495457797
H,0,0.6877096186,3.1607668198,0.6556421439
H,0,-0.6952282175,2.1879059779,1.1205526214

H,0,-0.2375269345,0.5700171359,-0.6923547447
H,0,-0.3558286115,2.1845076174,-1.3624708149
H,0,2.0871863224,2.4113606398,-1.4582645392
H,0,1.6099495134,0.9563562181,-2.3165894761
H,0,3.6339413952,0.7045546961,-0.8388032887
H,0,3.0284229977,-1.4712152984,0.1553579258
H,0,2.3422380054,-1.3057183909,-1.4644563877
H,0,1.309302902,-1.1341330262,-0.0464999144
H,0,3.1265539163,2.1604713806,0.9605953889
H,0,1.3759582226,3.0850578904,3.2551043797
H,0,1.878784727,1.2157749769,3.9389564725

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205366	E(Thermal)=	0.214404
E(SCF)=	-298.569936	DE(MP2)=	-1.292306
DE(CBS)=	-0.122138	DE(MP34)=	-0.095746
DE(CCSD)=	-0.038230	DE(Int)=	0.044232
DE(Empirical)=	-0.067237		
CBS-QB3 (0 K)=	-299.935995	CBS-QB3 Energy=	-299.926957
CBS-QB3 Enthalpy=	-299.926012	CBS-QB3 Free Energy=	-299.968879

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B3LYP/6-31+G**
E(RB+HF-LYP) = -300.645429469

Zero-point correction= 0.207248 (Hartree/Particle)
Thermal correction to Energy= 0.216098
Thermal correction to Enthalpy= 0.217043
Thermal correction to Gibbs Free Energy= 0.174779
Sum of electronic and ZPE= -300.438181
Sum of electronic and thermal Energies= -300.429331
Sum of electronic and thermal Enthalpies= -300.428387
Sum of electronic and thermal Free Energies= -300.470650

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.604	35.077	88.950

C,0,2.7066427022,1.2520469228,0.9565198036
H,0,3.3824321478,0.6996741825,1.6203531224
C,0,1.3369996175,1.4368019558,1.6499142704
C,0,0.2846727045,2.114598577,0.7281957958

C,0,0.2035794553,1.3909608935,-0.6348345637
C,0,1.5722472871,1.2340418081,-1.3185298538
C,0,2.581910739,0.5332647833,-0.3963196503
H,0,2.2508397661,-0.5018015899,-0.2222988711
B,0,1.3551294491,1.8930528829,3.1369925455
C,0,0.5473915677,3.623736139,0.5685370653
H,0,-0.6933628039,2.0130489958,1.2182966839
H,0,-0.2233796787,0.3901773057,-0.4742333396
H,0,-0.4921551897,1.9225318865,-1.2974627033
H,0,1.9637282082,2.2201782994,-1.6039350818
H,0,1.4571909011,0.6695207457,-2.2522743746
H,0,3.5627099269,0.4690395785,-0.884386281
H,0,3.1727044391,2.2348097849,0.7999345652
H,0,0.372902534,2.3552293778,3.6452768901
H,0,2.3133373403,1.6951685722,3.8288789045
H,0,0.9517628058,0.4045806897,1.854336215
H,0,0.5270039995,4.1283922179,1.5416499156
H,0,1.5183149397,3.833227805,0.1075158502
H,0,-0.2210678586,4.0872641857,-0.060977908

B3LYP/6-31G*
E(RB+HF-LYP) = -300.618289814

Zero-point correction= 0.208727 (Hartree/Particle)
Thermal correction to Energy= 0.217540
Thermal correction to Enthalpy= 0.218484
Thermal correction to Gibbs Free Energy= 0.176271
Sum of electronic and ZPE= -300.409561
Sum of electronic and thermal Energies= -300.400749
Sum of electronic and thermal Enthalpies= -300.399805
Sum of electronic and thermal Free Energies= -300.442017

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.511	34.785	88.873

C,0,2.7043742051,1.2498329915,0.9563661654
H,0,3.3818688981,0.6985842804,1.6202139704
C,0,1.3345369707,1.432152536,1.65000678
C,0,0.2842143623,2.1137964879,0.7288316517
C,0,0.2017955198,1.3900079578,-0.6334301359
C,0,1.5700092379,1.2330621478,-1.3167936145
C,0,2.5780629722,0.5303155742,-0.395201559

H,0,2.2445546897,-0.5041283301,-0.2203739216
B,0,1.3585501333,1.9014596328,3.1348624164
C,0,0.5516054506,3.6209913199,0.5686585955
H,0,-0.6944834232,2.0156192975,1.2191194798
H,0,-0.225480111,0.3889949819,-0.4725247043
H,0,-0.4942434748,1.9212742781,-1.2967431578
H,0,1.9625770838,2.2197934703,-1.600049594
H,0,1.4550790013,0.6701905957,-2.2520854246
H,0,3.5589424423,0.4630247775,-0.8837958781
H,0,3.16965078,2.2330962894,0.7987831137
H,0,0.3779531468,2.3677651672,3.6447535504
H,0,2.3210777954,1.7131017357,3.825054579
H,0,0.9490735149,0.3993961156,1.8475400819
H,0,0.5343104094,4.1262453196,1.5422807829
H,0,1.5233704895,3.8274932053,0.1064816059
H,0,-0.2158650942,4.0874761679,-0.0608057833

CBS-QB3

C,0,2.7108119662,1.2460646358,0.9499170178
H,0,3.3866311384,0.6914586118,1.6080967189
C,0,1.3452414154,1.4296537561,1.6487415313
C,0,0.2904880165,2.1096281923,0.733547205
C,0,0.2033945415,1.3900714481,-0.6293707157
C,0,1.5678366646,1.2351075154,-1.3180739008
C,0,2.5800107039,0.5322418729,-0.4030716354
H,0,2.25080045,-0.5014854351,-0.2312105722
B,0,1.370078349,1.8828067743,3.1334171646
C,0,0.5547542646,3.6167244296,0.5759029267
H,0,-0.6833094339,2.0071423101,1.2265481053
H,0,-0.2231688673,0.3913478102,-0.4698824604
H,0,-0.4931696647,1.9229989881,-1.2863124892
H,0,1.9574656949,2.219946911,-1.6022567632
H,0,1.4491818032,0.6742903825,-2.250960147
H,0,3.5567622536,0.4698603478,-0.8945080338
H,0,3.1769719531,2.2266673551,0.7955996416
H,0,0.3932203338,2.3457795034,3.6445438924
H,0,2.3297774057,1.6851807534,3.8183800752
H,0,0.9604818742,0.3982418538,1.8499729349
H,0,0.5379113284,4.1189786233,1.5481049783
H,0,1.5228980427,3.8252461951,0.1132873656

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.204702	E(Thermal)=	0.213633
E(SCF)=	-298.570195	DE(MP2)=	-1.292428

DE(CBS)=	-0.122154	DE(MP34)=	-0.095902
DE(CCSD)=	-0.038188	DE(Int)=	0.044239
DE(Empirical)=	-0.067222		
CBS-QB3 (0 K)=	-299.937148	CBS-QB3 Energy=	-299.928217
CBS-QB3 Enthalpy=	-299.927273	CBS-QB3 Free Energy=	-299.969680

4e-21
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.645206718

Zero-point correction= 0.207675 (Hartree/Particle)
Thermal correction to Energy= 0.216371
Thermal correction to Enthalpy= 0.217315
Thermal correction to Gibbs Free Energy= 0.175193
Sum of electronic and ZPE= -300.437532
Sum of electronic and thermal Energies= -300.428836
Sum of electronic and thermal Enthalpies= -300.427892
Sum of electronic and thermal Free Energies= -300.470013

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.775	34.626	88.652

C,0,-0.0243115674,0.2390091416,-0.0765174096
C,0,0.2450543026,0.0907059175,1.4299482571
C,0,1.7589184613,-0.0037851882,1.7200280903
C,0,2.4936093776,1.2342048477,1.1447450934
C,0,2.2613731748,1.3783775548,-0.3761845831
C,0,0.7451025438,1.4310242286,-0.6723284039
H,0,2.6964668788,2.338675617,-0.687597405
B,0,2.4438658676,-1.3760120856,1.4194003119
H,0,2.1211540851,2.1415340375,1.6416480215
H,0,1.9070980697,0.0225118405,2.8227729964
H,0,3.6344281553,-1.4764395615,1.5071031261
H,0,3.5684767154,1.1735765566,1.3557153773
H,0,1.8071774741,-2.3672929255,1.1965229597
H,0,-0.2739402102,-0.793378312,1.8197285934
H,0,-0.1785599082,0.9616678895,1.9529721278
C,0,2.9771748021,0.2813716308,-1.1793682591
H,0,0.577327076,1.4881918797,-1.7558055024
H,0,0.339333552,2.3595514117,-0.2455568143
H,0,-1.098962841,0.3651466252,-0.2577386116

H,0,0.2640425926,-0.6892211304,-0.5886549361
H,0,2.8135010506,0.4121352532,-2.255283834
H,0,4.0569679619,0.2973119299,-0.9969815082
H,0,2.6168603854,-0.7267071583,-0.9297536877

B3LYP/6-31G*
E(RB+HF-LYP) = -300.618283169

Zero-point correction= 0.209318 (Hartree/Particle)
Thermal correction to Energy= 0.217868
Thermal correction to Enthalpy= 0.218812
Thermal correction to Gibbs Free Energy= 0.177160
Sum of electronic and ZPE= -300.408965
Sum of electronic and thermal Energies= -300.400416
Sum of electronic and thermal Enthalpies= -300.399472
Sum of electronic and thermal Free Energies= -300.441123

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.715	34.227	87.690

C,0,-0.0254162991,0.2401766282,-0.0699007068
C,0,0.2456409395,0.0962464229,1.4362560383
C,0,1.7588925105,0.0015676804,1.7280393162
C,0,2.488967763,1.2422700081,1.1492404973
C,0,2.2614967113,1.3726681471,-0.372518114
C,0,0.7465994598,1.4266816953,-0.6720295032
H,0,2.7018755528,2.3271877705,-0.6951346092
B,0,2.45083415,-1.3592027967,1.3798694671
H,0,2.1085383846,2.1497945358,1.640660088
H,0,1.908248934,0.0322689995,2.8284032311
H,0,3.6390228047,-1.4650300315,1.4998019488
H,0,3.5637788271,1.1900367514,1.36527887
H,0,1.8249742533,-2.3381420261,1.0800412173
H,0,-0.2755395583,-0.7860636736,1.8286287775
H,0,-0.1770932068,0.9690303155,1.9578106255
C,0,2.9745195152,0.2619116781,-1.1572567785
H,0,0.57988913,1.4773984066,-1.7564584806
H,0,0.3424385016,2.359228976,-0.251604166
H,0,-1.1003924496,0.3688804865,-0.2500800246
H,0,0.2592454172,-0.6908400873,-0.5795357782
H,0,2.8111028916,0.3716266616,-2.2361341518
H,0,4.0547451153,0.2765182858,-0.9745880216
H,0,2.6097886524,-0.742054834,-0.8899757424

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200943	E(Thermal)=	0.209819
E(QCISD(T))=	-299.599640	E(Empiric)=	-0.155480
DE(Plus)=	-0.013439	DE(2DF)=	-0.300597
E(Delta-G3)=	-0.436056	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.304269	G3 Energy=	-300.295393
G3 Enthalpy=	-300.294449	G3 Free Energy=	-300.336676

CBS-QB3

C,0,-0.0218677325,0.2401406102,-0.0786994333
C,0,0.2463238142,0.090478584,1.4258940446
C,0,1.7586522574,-0.0049171772,1.7156512427
C,0,2.4962633943,1.2290603377,1.1406132872
C,0,2.2615139388,1.3776546803,-0.377861091
C,0,0.7464631878,1.4320712081,-0.6714811443
H,0,2.6947651689,2.3374306739,-0.6851640206
B,0,2.4395035049,-1.3787596057,1.4362481162
H,0,2.1301109551,2.1352682307,1.6392246421
H,0,1.9038277307,0.0261686329,2.8177448354
H,0,3.628194519,-1.4764154199,1.5137515389
H,0,3.5690392109,1.1628296197,1.3486782443
H,0,1.8014410253,-2.3714721059,1.2408540157
H,0,-0.2709692569,-0.7922858341,1.8144491017
H,0,-0.1759256483,0.9592099249,1.9490123917
C,0,2.9744452143,0.2850320533,-1.186165131
H,0,0.5781531801,1.49196189,-1.7524381393
H,0,0.3424807241,2.358036341,-0.2430640156
H,0,-1.0942526791,0.3660131424,-0.2598555185
H,0,0.2661904166,-0.6855219889,-0.5912449508
H,0,2.8121824504,0.4241059361,-2.2592045752
H,0,4.0522617273,0.2984812757,-1.0037651759

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205102	E(Thermal)=	0.213890
E(SCF)=	-298.569602	DE(MP2)=	-1.294341
DE(CBS)=	-0.122180	DE(MP34)=	-0.095642
DE(CCSD)=	-0.038286	DE(Int)=	0.044243
DE(Empirical)=	-0.067196		
CBS-QB3 (0 K)=	-299.937902	CBS-QB3 Energy=	-299.929115
CBS-QB3 Enthalpy=	-299.928170	CBS-QB3 Free Energy=	-299.970459

4e-22
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.644746522

Zero-point correction= 0.207575 (Hartree/Particle)
Thermal correction to Energy= 0.216324
Thermal correction to Enthalpy= 0.217268
Thermal correction to Gibbs Free Energy= 0.175213
Sum of electronic and ZPE= -300.437171
Sum of electronic and thermal Energies= -300.428423
Sum of electronic and thermal Enthalpies= -300.427479
Sum of electronic and thermal Free Energies= -300.469533

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.745	34.843	88.511

C,0,2.3249072553,0.8804416358,-0.2360501444
C,0,2.504157914,0.3693297401,1.212677025
C,0,1.1377281818,0.4391155003,1.9484906739
C,0,0.0286605898,-0.3332017967,1.1966528555
C,0,-0.1256732451,0.1996279687,-0.2374174295
C,0,1.2070033062,0.151145455,-1.0014868632
B,0,0.7291480475,1.8392357037,2.498430266
C,0,3.1526006665,-1.0258733647,1.2617186585
H,0,0.2630262902,-1.4058056054,1.1555159068
H,0,1.2693849142,-0.0410961151,2.9500196098
H,0,-0.4139904823,2.0811983912,2.7652765559
H,0,-0.9206390048,-0.2419709879,1.7373714281
H,0,1.5613524764,2.6590334558,2.7671738758
H,0,3.1909532863,1.0593178597,1.7211087452
H,0,-0.8928890084,-0.3710169316,-0.775406867
H,0,-0.4827900435,1.2404134406,-0.1967376777
H,0,1.0896811452,0.5950269064,-1.9979494394
H,0,1.4915461677,-0.8972711144,-1.1649632736
H,0,3.2738378433,0.7954623795,-0.7813520437
H,0,2.0837409048,1.953516184,-0.1989022481
H,0,4.1265267787,-1.0183890593,0.758127016
H,0,3.3171231564,-1.3428889908,2.2982767308
H,0,2.5397788598,-1.7929146548,0.7773496389

B3LYP/6-31G*
E(RB+HF-LYP) = -300.617640256

Zero-point correction= 0.209058 (Hartree/Particle)
Thermal correction to Energy= 0.217768
Thermal correction to Enthalpy= 0.218712
Thermal correction to Gibbs Free Energy= 0.176718
Sum of electronic and ZPE= -300.408546
Sum of electronic and thermal Energies= -300.399837
Sum of electronic and thermal Enthalpies= -300.398892
Sum of electronic and thermal Free Energies= -300.440887

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.649	34.548	88.403

C,0,2.323878671,0.8820154217,-0.2320549703
C,0,2.5047370208,0.3683859506,1.21487029
C,0,1.1391449737,0.4364230838,1.9525354458
C,0,0.0312155221,-0.3362388052,1.1999620588
C,0,-0.1243107914,0.197839862,-0.2327010533
C,0,1.207522144,0.1512784079,-0.9971632551
B,0,0.7273460733,1.8440924776,2.4857738345
C,0,3.1515903122,-1.0266403515,1.2603164107
H,0,0.2667010803,-1.4090107287,1.1582008337
H,0,1.2720775241,-0.0466595388,2.9516634878
H,0,-0.4178300508,2.0907532009,2.7439142924
H,0,-0.9186606062,-0.2465647424,1.7408852806
H,0,1.5580261087,2.6686483231,2.7488695966
H,0,3.1928599418,1.0570664808,1.7241233466
H,0,-0.8922247915,-0.3722025735,-0.7712647047
H,0,-0.4818243633,1.238866753,-0.1901433009
H,0,1.0891862401,0.5945962413,-1.9942764788
H,0,1.4938907938,-0.8971084526,-1.160187069
H,0,3.2726593245,0.8009323519,-0.7790815371
H,0,2.0795883863,1.9548418549,-0.1926397329
H,0,4.1260280742,-1.0192189763,0.7565261078
H,0,3.3155853048,-1.3473589698,2.2964095211
H,0,2.5379891071,-1.7923012708,0.7733845957

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200689	E(Thermal)=	0.209724
E(QCISD(T))=	-299.598101	E(Empiric)=	-0.155480
DE(Plus)=	-0.013572	DE(2DF)=	-0.300477
E(Delta-G3)=	-0.435901	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.302843	G3 Energy=	-300.293807
G3 Enthalpy=	-300.292863	G3 Free Energy=	-300.335436

CBS-QB3

C,0,2.3253191761,0.880418728,-0.2336458951
C,0,2.5025501078,0.3693059452,1.2134195746
C,0,1.1367715987,0.4397162563,1.9475662995
C,0,0.029399307,-0.3317684447,1.195582479
C,0,-0.1226547838,0.1992662345,-0.2374897967
C,0,1.2094641759,0.1516667448,-0.9992252947
B,0,0.7298152612,1.8371420645,2.4962899193
C,0,3.1482981727,-1.0249943664,1.2619937481
H,0,0.2627143786,-1.4024727148,1.1572421093
H,0,1.2681896651,-0.0430784491,2.9460693608
H,0,-0.4110542624,2.0801902002,2.7593388087
H,0,-0.9182961817,-0.2389586691,1.7342270329
H,0,1.561155464,2.653981586,2.7639665963
H,0,3.1868752174,1.0576216637,1.7222995632
H,0,-0.8868963349,-0.3713835045,-0.7750851257
H,0,-0.4805493986,1.2376676715,-0.198547966
H,0,1.0929151805,0.5952266351,-1.9934497545
H,0,1.4942417866,-0.8943351633,-1.1633240927
H,0,3.2729036218,0.7951752861,-0.7766564102
H,0,2.0853965572,1.9516358651,-0.1969781322
H,0,4.1217697675,-1.0176063203,0.7618538456
H,0,3.3097933868,-1.3427055924,2.2966537661

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205033	E(Thermal)=	0.213862
E(SCF)=	-298.569383	DE(MP2)=	-1.293150
DE(CBS)=	-0.122148	DE(MP34)=	-0.095777
DE(CCSD)=	-0.038220	DE(Int)=	0.044242
DE(Empirical)=	-0.067213		
CBS-QB3 (0 K)=	-299.936616	CBS-QB3 Energy=	-299.927788
CBS-QB3 Enthalpy=	-299.926844	CBS-QB3 Free Energy=	-299.969032

4e-23

B3LYP/6-31G*
E(RB+HF-LYP) = -300.582080471

Zero-point correction= 0.203437 (Hartree/Particle)
Thermal correction to Energy= 0.213594
Thermal correction to Enthalpy= 0.214538
Thermal correction to Gibbs Free Energy= 0.167457

Sum of electronic and ZPE= -300.378644
Sum of electronic and thermal Energies= -300.368487
Sum of electronic and thermal Enthalpies= -300.367543
Sum of electronic and thermal Free Energies= -300.414623

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.032	36.677	99.089

C,0,0.,0.,0.
C,0,0.,0.,1.515898
C,0,1.111893,0.,2.268742
B,0,-0.448576,2.720565,2.933063
H,0,-0.97389,-0.048319,2.003547
C,0,2.50625,0.033172,1.691792
H,0,1.023264,-0.056671,3.353218
H,0,-1.02232,2.141511,3.806592
H,0,-1.016542,2.972219,1.912821
H,0,0.65512,3.137057,3.11915
H,0,3.129818,0.731036,2.266543
H,0,2.97122,-0.956554,1.82802
C,0,-1.066373,-0.960433,-0.552782
H,0,-0.268556,1.014786,-0.336292
C,0,1.399408,-0.333797,-0.552176
H,0,1.437725,-0.101969,-1.624087
C,0,2.504027,0.415189,0.203346
H,0,1.569203,-1.416899,-0.459447
H,0,3.484733,0.207771,-0.24162
H,0,2.336642,1.496972,0.109934
H,0,-1.08214,-0.935936,-1.648826
H,0,-0.863916,-1.992462,-0.241307
H,0,-2.068293,-0.692809,-0.196767

G8_3methylcyclohexene_eq_trans_3.206
ohexene_eq_trans_3.206 3B3
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.610234910

Zero-point correction= 0.202181 (Hartree/Particle)
Thermal correction to Energy= 0.212250
Thermal correction to Enthalpy= 0.213194
Thermal correction to Gibbs Free Energy= 0.166753
Sum of electronic and zero-point Energies= -300.408054
Sum of electronic and thermal Energies= -300.397985

Sum of electronic and thermal Enthalpies= -300.397041
Sum of electronic and thermal Free Energies= -300.443482

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.195299 E(Thermal)= 0.205760
E(QCISD(T))= -299.560126 E(Empiric)= -0.155480
DE(Plus)= -0.015674 DE(2DF)= -0.296684
E(Delta-G3)= -0.435296 E(G3-Empiric)= -0.155480
G3(0 K)= -300.267961 G3 Energy= -300.257500
G3 Enthalpy= -300.256556 G3 Free Energy= -300.304245

4e-24
B3LYP/6-31+G**
E(RB+HF-LYP) = -300.611285113
Zero-point correction= 0.202924 (Hartree/Particle)
Thermal correction to Energy= 0.212604
Thermal correction to Enthalpy= 0.213548
Thermal correction to Gibbs Free Energy= 0.168601
Sum of electronic and zero-point Energies= -300.408361
Sum of electronic and thermal Energies= -300.398681
Sum of electronic and thermal Enthalpies= -300.397737
Sum of electronic and thermal Free Energies= -300.442684

B3LYP/6-31G*
E(RB+HF-LYP) = -300.583637531

Zero-point correction= 0.204203 (Hartree/Particle)
Thermal correction to Energy= 0.213945
Thermal correction to Enthalpy= 0.214889
Thermal correction to Gibbs Free Energy= 0.169510
Sum of electronic and ZPE= -300.379435
Sum of electronic and thermal Energies= -300.369692
Sum of electronic and thermal Enthalpies= -300.368748
Sum of electronic and thermal Free Energies= -300.414127

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.253	36.164	95.508

C,0,0.613926,-0.099326,-0.881296
H,0,1.523629,-0.010207,-1.475576

C,0,0.094019,-1.318126,-0.650258
C,0,-1.213542,-1.539017,0.07482
C,0,-2.028995,-0.241232,0.200436
C,0,-1.131871,0.932197,0.613202
C,0,-0.029895,1.195027,-0.429273
H,0,-0.506394,1.639228,-1.320777
B,0,2.632757,-1.434854,0.752037
H,0,-1.012404,-1.959876,1.071546
H,0,-1.795332,-2.305157,-0.455213
H,0,-2.497798,-0.013521,-0.766922
H,0,-2.844563,-0.376955,0.920889
H,0,-0.660546,0.706788,1.580977
H,0,-1.72695,1.842545,0.75771
C,0,1.011534,2.205629,0.075829
H,0,3.235919,-1.577765,-0.269705
H,0,2.719819,-0.408118,1.355798
H,0,2.081406,-2.369766,1.251243
H,0,0.597437,-2.196375,-1.046526
H,0,0.532949,3.154615,0.34561
H,0,1.531489,1.821677,0.960703
H,0,1.766507,2.416245,-0.690703

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.196035	E(Thermal)=	0.206088
E(QCISD(T))=	-299.561809	E(Empiric)=	-0.155480
DE(Plus)=	-0.015240	DE(2DF)=	-0.297197
E(Delta-G3)=	-0.435424	E(G3-Empiric)=	-0.155480
G3(0 K)=	-300.269116	G3 Energy=	-300.259063
G3 Enthalpy=	-300.258118	G3 Free Energy=	-300.304097

	Structure	CCSD(T)/6-311+G**
Starting material	4e-2	-273.2684378
	4e-1	-273.2694275
Complex	4e-6	-299.8055635
	4e-4	-299.8053248
	4e-5	-299.8071301
	4e-3	-299.8023605
Transition State	4e-13	-299.8012363
	4e-14	-299.8015548
	4e-11	-299.8023599
	4e-12	-299.8016924

	4e-9	-299.8041547
	4e-10	-299.8038297
	4e-11	-299.803887
	4e-12	-299.8039367
Product	4e-22	-299.8358292
	4e-20	-299.8361856
	4e-21	-299.8371417
	4e-19	-299.835565
	4e-16	-299.8370246
	4e-18	-299.8386433
	4e-15	-299.8386433
	4e-17	-299.8381497
	Structure	M05/6-31+G**
Starting material	4e-2	-273.7503492
	4e-1	-273.7516495
Complex	4e-5	-300.3463822
	4e-6	-300.3460612
	4e-4	-300.3479364
	4e-3	-300.3483736
Transition State	4e-13	-300.3488591
	4e-14	-300.3491072
	4e-11	-300.3501468
	4e-12	-300.3495638
	4e-9	-300.3520137
	4e-10	-300.3518087
	4e-7	-300.3518526
	4e-8	-300.3520636

	Structure	CCSD(T)/6-31+G**
Starting Material	4e-2	-273.1796904
	4e-1	-273.1808604
Complex	4e-6	-299.703862
	4e-4	-299.7058181
	4e-5	-299.705797
	c4e-3	-299.7072322
Transition State	4e-13	-299.699546
	4e-14	-299.6998824
	4e-11	-299.7002049
	4e-12	-299.7002049

	4e-9	-299.7026828
	4e-10	-299.7023622
	4e-7	-299.7024361
	4e-8	-299.7025529
	4e-20	-299.7353207
	4e-21	-299.699546
	4e-22	-299.6998824
Product	4e-19	-299.7009498
	4e-16	-299.7002049
	4e-17	-299.7026828
	4e-18	-299.7023622
	4e-15	-299.7026828

	Structure	CCSD(T)/aug-cc-pvdz
Starting Material	4e-1	-273.2145776
	4e-2	-273.2155208
	4e-6	-299.7472297
Complex	4e-4	-299.7465815
	4e-5	-299.7486779
	4e-3	-299.7435774
	4e-13	-299.7419117
	4e-14	-299.7423506
	4e-11	-299.7426792
Transition State	4e-12	-299.7421989
	4e-9	-299.7445118
	4e-10	-299.7445106
	4e-7	-299.7442834
	4e-8	-299.7442072

	Structure	CCSD(T)/aug-cc-pvdz
Product	4e-22	-299.7774175
	4e-20	-299.7775673
	4e-21	-299.7791591
	4e-19	-299.7768561
	4e-16	-299.7788615
	4e-18	-299.7800281
	4e-15	-299.7802816
	4e-17	-299.7796326

	Structure	MPWPW91/6-311+G**
Starting material	4e-2	-273.9243659

	4e-1	-273.925548
Complex	4e-3	-300.5505955
	4e-6	-300.5479734
	4e-5	-300.5489053
	4e-4	-300.5498132
Transition State	4e-8	-300.5504626
	4e-14	-300.5474104
	4e-14	-300.5479742
	4e-11	-300.5487031
	4e-12	-300.5481247
	4e-9	-300.5504163
	4e-10	-300.5504061
	4e-7	-300.5503223
	Structure	TPSSTPSS/cc-pvtz
Starting material	4e-2	-274.0995472
	4e-1	-274.17102
Complex	4e-3	-300.7490552
	4e-6	-300.7460945
	4e-4	-300.7478815
	4e-5	-300.7472459
Transition State	4e-13	-300.7426341
	4e-14	-300.7431238
	4e-11	-300.7437081
	4e-12	-300.7430395
	4e-9	-300.7452494
	4e-10	-300.7451997
	4e-7	-300.7451306
	4e-8	-300.7452246
	Structure	CCSD(T)/cc-pvdz
Starting material	4e-2	-273.1660598
	4e-1	-273.1670782
Complex	4e-5	-299.6937695
	4e-6	-299.6907909
	4e-4	-299.6924497
	4e-3	-299.6937695
Transition State	4e-13	-299.6862329
	4e-14	-299.6865944
	4e-11	-299.6872404

	4e-12	-299.6866746
	4e-9	-299.6889962
	4e-10	-299.6889564
	4e-7	-299.6889071
	4e-8	-299.6888685

	Structure	MP4(sdq)/aug-cc-pvdz
Starting material	4e-2	-273.1729457
	4e-1	-273.1739494
Complex	4e-6	-299.6891517
	4e-4	-299.69076
	4e-5	-299.6906185
	4e-3	-299.6920108
Transition State	4e-11	-299.6953369
	4e-13	-299.6944995
	4e-12	-299.6948988
	4e-9	-299.6971429
	4e-10	-299.6971705
	4e-7	-299.697022
	4e-8	-299.6969218
	4e-14	-299.6949001
Product	4e-22	-299.7335662
	4e-20	-299.7337797
	4e-21	-299.7351726
	4e-19	-299.733025
	4e-16	-299.7349937
	4e-18	-299.7361318
	4e-15	-299.7365408
	4e-17	-299.7358581

	Structure	MP4(sdtq)/cc-pvtz
Starting material	4e-2	-273.1231325
	4e-1	-273.1650628
Complex	4e-6	-299.6891517
	4e-4	-299.69076
	4e-5	-299.6906185
	4e-3	-299.6920108
Transition State	4e-13	-299.6851405
	4e-14	-299.6855224
	4e-11	-299.6861633

	4e-12	-299.6855676
	4e-9	-299.6879291
	4e-10	-299.6878256
	4e-7	-299.6877660
	4e-8	-299.6877397
	4e-22	-299.7204313
	4e-20	-299.7206347
	4e-21	-299.7218531
	4e-19	-299.7198575
Product	4e-16	-299.7216558
	4e-18	-299.7228788
	4e-15	-299.7232939
	4e-17	-299.7225881
	Structure	MPWLYP/6-31+G**
Starting material	4e-2	-273.9835646
	4e-1	-273.9848743
	4e-3	-300.6150726
	4e-6	-300.6117803
Complex	4e-4	-300.6138796
	4e-5	-300.6133474
	Structure	MPWLYP/6-31+G**
	4e-13	-300.6076049
	4e-14	-300.6078724
	4e-11	-300.6087227
	4e-12	-300.6081492
Transition State	4e-9	-300.615492
	4e-10	-300.6107074
	4e-7	-300.6107127
	4e-8	-300.6106478

A. 4. Theoretical Structures from "Dynamics and Selectivity In The Hydroboration of Alkenes *Via* Chloroborane"

Propene
B3LYP/6-31+G**
E(RB+HF-LYP) = -117.922799177

Zero-point correction= 0.079556 (Hartree/Particle)
Thermal correction to Energy= 0.083653
Thermal correction to Enthalpy= 0.084597
Thermal correction to Gibbs Free Energy= 0.054531
Sum of electronic and ZPE= -117.843243
Sum of electronic and thermal Energies= -117.839146
Sum of electronic and thermal Enthalpies= -117.838202
Sum of electronic and thermal Free Energies= -117.868268

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	52.493	13.015	63.280

C,0,0.0344608581,-0.1196186007,-0.0253367535
H,0,-0.7225196876,0.6145938205,-0.3292384394
C,0,0.0641536597,-0.2773363759,1.4684961103
C,0,1.1264931839,-0.0522279939,2.2475837269
H,0,-0.229463632,-1.0649677664,-0.5163525082
H,0,-0.8672370321,-0.6026054777,1.9338697675
H,0,2.0784454947,0.2734473875,1.833158635
H,0,1.0819141746,-0.1852657575,3.324646825
H,0,1.0037429807,0.2082407643,-0.4141473637

B3LYP/6-31G*
E(RB+HF-LYP) = -117.907556179

Zero-point correction= 0.080081 (Hartree/Particle)
Thermal correction to Energy= 0.084158
Thermal correction to Enthalpy= 0.085102
Thermal correction to Gibbs Free Energy= 0.055079
Sum of electronic and ZPE= -117.827475
Sum of electronic and thermal Energies= -117.823398
Sum of electronic and thermal Enthalpies= -117.822454
Sum of electronic and thermal Free Energies= -117.852477

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	52.810	12.917	63.189

C,0,0.0345565707,-0.1197608226,-0.0234351422
H,0,-0.7220376636,0.6151139371,-0.330185343
C,0,0.0640978356,-0.277641459,1.4700545078
C,0,1.1246474375,-0.0526175058,2.2461570925
H,0,-0.2287854144,-1.0648944572,-0.5174128732
H,0,-0.8686000739,-0.6030047319,1.9335519938
H,0,2.0769329525,0.2730371984,1.8315449994
H,0,1.084559352,-0.1842527935,3.3241654131
H,0,1.0046190036,0.2082806345,-0.4117606481

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.076878	E(Thermal)=	0.081041
E(QCISD(T))=	-117.508195	E(Empiric)=	-0.060840
DE(Plus)=	-0.007429	DE(2DF)=	-0.116313
E(Delta-G3)=	-0.168940	E(G3-Empiric)=	-0.060840
G3(0 K)=	-117.784839	G3 Energy=	-117.780675
G3 Enthalpy=	-117.779731	G3 Free Energy=	-117.809894

For Anharmonic Corrections of Propene

Zero-point vibrational energy 210198.2 (Joules/Mol)
50.23857 (Kcal/Mol)
Warning -- explicit consideration of 3 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 289.91 609.04 843.87 1339.89 1340.38
(Kelvin) 1372.37 1485.77 1554.10 1730.75 1922.49
2060.80 2115.88 2170.59 2190.64 2484.78
4373.25 4443.46 4492.28 4530.66 4546.95
4664.16

Zero-point correction=	0.080060 (Hartree/Particle)
Thermal correction to Energy=	0.084155
Thermal correction to Enthalpy=	0.085099
Thermal correction to Gibbs Free Energy=	0.055030
Sum of electronic and zero-point Energies=	-117.827479
Sum of electronic and thermal Energies=	-117.823384
Sum of electronic and thermal Enthalpies=	-117.822440
Sum of electronic and thermal Free Energies=	-117.852509

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	52.808	12.955	63.285

ZPE(harm) = 0.21020D+03 kJ/mol ZPE(anh)= 0.20739D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.30971D-36	0.10555D-35	
QZvib	0.20703D+01	0.22735D+01	
Energy	0.22095D+03	0.21831D+03	kJ/mol
Enthalpy	0.22343D+03	0.22079D+03	kJ/mol
Entropy	0.26478D+03	0.26612D+03	J/(mol K)
Sp.Heat(V)	0.54204D+02	0.55064D+02	J/(mol K)
Sp.Heat(P)	0.62518D+02	0.63378D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.30971D-36	0.10555D-35	
QZvib	0.20703D+01	0.22735D+01	
Energy	0.22095D+03	0.21831D+03	kJ/mol
Enthalpy	0.22343D+03	0.22079D+03	kJ/mol
Entropy	0.26478D+03	0.26612D+03	J/(mol K)
Sp.Heat(V)	0.54204D+02	0.55064D+02	J/(mol K)
Sp.Heat(P)	0.62518D+02	0.63378D+02	J/(mol K)

5a-1 Starting Material

B3LYP/6-31+G**

E(RB+HF-LYP) = -486.273583244

Zero-point correction= 0.021231 (Hartree/Particle)
Thermal correction to Energy= 0.024247
Thermal correction to Enthalpy= 0.025191
Thermal correction to Gibbs Free Energy= -0.001420
Sum of electronic and ZPE= -486.252353
Sum of electronic and thermal Energies= -486.249336
Sum of electronic and thermal Enthalpies= -486.248392
Sum of electronic and thermal Free Energies= -486.275003

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	15.215	7.675	56.007

B,0,0.0286818035,0.,0.0165590057
H,0,-0.013517952,0.,1.2037700412
H,0,1.035737452,0.,-0.6135915978
Cl,0,-1.4891412615,0.,-0.8597575287

B3LYP/6-31G*
E(RB+HF-LYP) = -486.269584918

Zero-point correction= 0.021358 (Hartree/Particle)
Thermal correction to Energy= 0.024371
Thermal correction to Enthalpy= 0.025315
Thermal correction to Gibbs Free Energy= -0.001292
Sum of electronic and ZPE= -486.248227
Sum of electronic and thermal Energies= -486.245214
Sum of electronic and thermal Enthalpies= -486.244270
Sum of electronic and thermal Free Energies= -486.270877

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	15.293	7.655	55.999

B,0,0.0274450109,0.,0.0158449422
H,0,-0.0126651868,0.,1.2043818933
H,0,1.0366937139,0.,-0.6131590067
Cl,0,-1.4897134952,0.,-0.8600879087

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.020504	E(Thermal)=	0.023543
E(QCISD(T))=	-485.587266	E(Empiric)=	-0.040560
DE(Plus)=	-0.002846	DE(2DF)=	-0.087858
E(Delta-G3)=	-0.393016	E(G3-Empiric)=	-0.040560
G3(0 K)=	-486.091042	G3 Energy=	-486.088002
G3 Enthalpy=	-486.087058	G3 Free Energy=	-486.113700

For Anharmonic Corrections of 5a-1

Zero-point vibrational energy 56125.0 (Joules/Mol)
13.41419 (Kcal/Mol)
Vibrational temperatures: 1178.16 1268.67 1440.26 1784.04 3832.19
(Kelvin) 3997.24

Zero-point correction= 0.021377 (Hartree/Particle)

Thermal correction to Energy= 0.024391
Thermal correction to Enthalpy= 0.025336
Thermal correction to Gibbs Free Energy= -0.001273
Sum of electronic and zero-point Energies= -486.248206
Sum of electronic and thermal Energies= -486.245191
Sum of electronic and thermal Enthalpies= -486.244247
Sum of electronic and thermal Free Energies= -486.270856

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	15.306	7.665	56.003
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	37.530
Rotational	0.889	2.981	18.002
Vibrational	13.528	1.703	0.471

	Q	Log10(Q)	Ln(Q)
Total Bot	0.385157D+01	0.585637	1.348480

ZPE(harm) = 0.56125D+02 kJ/mol ZPE(anh)= 0.55457D+02 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.15366D-09	0.20164D-09	
QZvib	0.10452D+01	0.10475D+01	
Energy	0.64040D+02	0.63389D+02	kJ/mol
Enthalpy	0.66519D+02	0.65868D+02	kJ/mol
Entropy	0.23432D+03	0.23439D+03	J/(mol K)
Sp.Heat(V)	0.32070D+02	0.32262D+02	J/(mol K)
Sp.Heat(P)	0.40384D+02	0.40576D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.15366D-09	0.20164D-09	
QZvib	0.10452D+01	0.10475D+01	
Energy	0.64040D+02	0.63389D+02	kJ/mol
Enthalpy	0.66519D+02	0.65868D+02	kJ/mol
Entropy	0.23432D+03	0.23439D+03	J/(mol K)
Sp.Heat(V)	0.32070D+02	0.32262D+02	J/(mol K)
Sp.Heat(P)	0.40384D+02	0.40576D+02	J/(mol K)

5a-2 Complex
B3LYP/6-31+G**

E(RB+HF-LYP) = -604.198568365

Zero-point correction= 0.104920 (Hartree/Particle)
Thermal correction to Energy= 0.112137
Thermal correction to Enthalpy= 0.113081
Thermal correction to Gibbs Free Energy= 0.073613
Sum of electronic and ZPE= -604.093648
Sum of electronic and thermal Energies= -604.086432
Sum of electronic and thermal Enthalpies= -604.085487
Sum of electronic and thermal Free Energies= -604.124955

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.367	24.383	83.067

C,0,-0.0908072736,0.0626445188,0.8891250108
B,0,0.2933758091,1.8567834637,1.7710695661
C,0,1.0505440951,-0.1673510389,1.598483336
C,0,2.4477084133,-0.0981905992,1.061282688
H,0,-0.0568568261,0.3336655935,-0.1615372526
H,0,-1.0579622202,-0.216801425,1.2897547774
H,0,0.9499106184,-0.5433305416,2.6145563672
H,0,0.8825106772,1.7839608421,2.8093484707
H,0,-0.8855977126,2.014748734,1.8721127297
Cl,0,1.1132108463,2.9136368759,0.5138308194
H,0,3.1017955325,0.4750262878,1.7252420491
H,0,2.8452420936,-1.1199533301,1.0092669865
H,0,2.4839059471,0.3434206189,0.0642844517

B3LYP/6-31G*
E(RB+HF-LYP) = -604.182476448

Zero-point correction= 0.105601 (Hartree/Particle)
Thermal correction to Energy= 0.112800
Thermal correction to Enthalpy= 0.113744
Thermal correction to Gibbs Free Energy= 0.074290
Sum of electronic and ZPE= -604.076875
Sum of electronic and thermal Energies= -604.069677
Sum of electronic and thermal Enthalpies= -604.068733
Sum of electronic and thermal Free Energies= -604.108186

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.783	24.239	83.038

C,0,-0.0903764544,0.0571111008,0.8894873233
B,0,0.2955803959,1.8649172509,1.7739866495
C,0,1.0496550012,-0.1705386647,1.598503052
C,0,2.4464315717,-0.0990559114,1.060206689
H,0,-0.0571099549,0.3293397681,-0.1612169291
H,0,-1.0594757577,-0.2184139846,1.2897718406
H,0,0.9500614578,-0.5449353913,2.6155917721
H,0,0.8816386392,1.7895472355,2.8148217787
H,0,-0.8860833866,2.0161062942,1.8678316799
Cl,0,1.1185372199,2.9123081887,0.5143882103
H,0,3.0995685667,0.4767222547,1.7237753156
H,0,2.8489993666,-1.1195679749,1.0062083165
H,0,2.4795533346,0.3447198338,0.0634643015

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101377	E(Thermal)=	0.108756
E(QCISD(T))=	-603.101241	E(Empiric)=	-0.101400
DE(Plus)=	-0.009410	DE(2DF)=	-0.209038
E(Delta-G3)=	-0.561154	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.880865	G3 Energy=	-603.873487
G3 Enthalpy=	-603.872543	G3 Free Energy=	-603.912358

For Anharmonic Corrections of 5a-2

Zero-point vibrational energy 277298.1 (Joules/Mol)
66.27584 (Kcal/Mol)
Warning -- explicit consideration of 7 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 101.08 156.80 261.63 321.53 401.13
(Kelvin) 508.05 612.81 941.80 970.36 1134.09
1319.40 1345.84 1379.23 1457.23 1510.10
1527.91 1567.60 1689.08 1751.07 1922.83
2060.31 2114.94 2163.21 2184.77 2375.12
3746.98 3835.29 4399.26 4492.43 4559.61
4584.43 4590.13 4716.51

Zero-point correction=	0.105617 (Hartree/Particle)
Thermal correction to Energy=	0.112832
Thermal correction to Enthalpy=	0.113777
Thermal correction to Gibbs Free Energy=	0.074253
Sum of electronic and zero-point Energies=	-604.076850
Sum of electronic and thermal Energies=	-604.069635

Sum of electronic and thermal Enthalpies= -604.068691
Sum of electronic and thermal Free Energies= -604.108214

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.803	24.269	83.184

ZPE(harm) = 0.27730D+03 kJ/mol ZPE(anh)= 0.27130D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.13085D-46	0.53361D-45	
QZvib	0.49801D+02	0.18080D+03	
Energy	0.29624D+03	0.28836D+03	kJ/mol
Enthalpy	0.29872D+03	0.29084D+03	kJ/mol
Entropy	0.34804D+03	0.36906D+03	J/(mol K)
Sp.Heat(V)	0.10154D+03	0.89422D+02	J/(mol K)
Sp.Heat(P)	0.10986D+03	0.97736D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.13085D-46	0.53361D-45	
QZvib	0.49801D+02	0.18080D+03	
Energy	0.29624D+03	0.28836D+03	kJ/mol
Enthalpy	0.29872D+03	0.29084D+03	kJ/mol
Entropy	0.34804D+03	0.36906D+03	J/(mol K)
Sp.Heat(V)	0.10154D+03	0.89422D+02	J/(mol K)
Sp.Heat(P)	0.10986D+03	0.97736D+02	J/(mol K)

5a-3 Complex
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.199332389

Zero-point correction= 0.105097 (Hartree/Particle)
Thermal correction to Energy= 0.112096
Thermal correction to Enthalpy= 0.113040
Thermal correction to Gibbs Free Energy= 0.074347
Sum of electronic and ZPE= -604.094236
Sum of electronic and thermal Energies= -604.087237
Sum of electronic and thermal Enthalpies= -604.086292
Sum of electronic and thermal Free Energies= -604.124985

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.341	24.223	81.436

C,0,-0.2041571284,-0.259239514,-0.284782765
C,0,-0.1181237612,-0.3200169958,1.2135139431
C,0,1.050109922,-0.2640982828,1.9198677424
B,0,0.1953352105,1.4997540239,2.1329569576
H,0,1.2897838728,1.9841335964,2.150330036
H,0,-0.4749892346,1.8995852976,1.2271917843
H,0,-1.0721606802,0.3162889149,-0.616350956
H,0,-0.315924399,-1.2810826302,-0.669737401
H,0,-1.0327993158,-0.5706086881,1.7460040015
H,0,1.9981250203,-0.1389152308,1.4055973638
H,0,1.0956477031,-0.5395113221,2.966975361
Cl,0,-0.6826601537,1.484184855,3.7558883087
H,0,0.6982629441,0.1725959763,-0.7258543766

B3LYP/6-31G*
E(RB+HF-LYP) = -604.183012671

Zero-point correction= 0.105758 (Hartree/Particle)
Thermal correction to Energy= 0.112757
Thermal correction to Enthalpy= 0.113701
Thermal correction to Gibbs Free Energy= 0.074970
Sum of electronic and ZPE= -604.077255
Sum of electronic and thermal Energies= -604.070256
Sum of electronic and thermal Enthalpies= -604.069312
Sum of electronic and thermal Free Energies= -604.108042

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.756	24.094	81.515

C,0,0.0662540358,-0.0974739534,1.1404904649
C,0,1.302188493,-0.0348495473,1.7148062963
C,0,2.592710518,-0.0041838429,0.9470622158
B,0,0.2865781576,1.7776740734,1.7503830061
H,0,1.3951922605,2.2294352421,1.7406775232
H,0,-0.0388898423,-0.1038218101,0.0592474788
H,0,-0.8188317516,-0.3426333809,1.7164906729
H,0,1.379015913,-0.1554011896,2.7930968922
Cl,0,-0.5653681945,1.9139849102,3.3784736856
H,0,-0.3638626595,2.1111717185,0.8018168318

H,0,3.3174636933,0.6749792841,1.4046347441
H,0,3.0309441157,-1.0112949494,0.9535632732
H,0,2.438305261,0.2916334453,-0.094783085

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101487	E(Thermal)=	0.108706
E(QCISD(T))=	-603.101840	E(Empiric)=	-0.101400
DE(Plus)=	-0.009611	DE(2DF)=	-0.208905
E(Delta-G3)=	-0.560826	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.881095	G3 Energy=	-603.873876
G3 Enthalpy=	-603.872932	G3 Free Energy=	-603.912133

For Anharmonic Corrections of 5a-3

Zero-point vibrational energy 277756.9 (Joules/Mol)
66.38550 (Kcal/Mol)
Warning -- explicit consideration of 7 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 142.59 219.34 268.11 344.49 420.88
(Kelvin) 567.93 618.27 903.13 961.62 1138.19
1331.88 1347.01 1380.63 1469.36 1512.98
1525.20 1566.39 1676.58 1741.78 1915.94
2058.29 2112.86 2166.64 2186.85 2360.79
3739.00 3811.46 4396.43 4493.36 4538.12
4581.65 4599.11 4716.02

Zero-point correction=	0.105792 (Hartree/Particle)
Thermal correction to Energy=	0.112790
Thermal correction to Enthalpy=	0.113734
Thermal correction to Gibbs Free Energy=	0.075004
Sum of electronic and zero-point Energies=	-604.077197
Sum of electronic and thermal Energies=	-604.070199
Sum of electronic and thermal Enthalpies=	-604.069255
Sum of electronic and thermal Free Energies=	-604.107984

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.777	24.111	81.513

ZPE(harm) = 0.27776D+03 kJ/mol ZPE(anh)= 0.27403D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00
Harmonic value SPT anharmonic value

Qvib	0.57811D-47	0.49820D-46	
QZvib	0.26477D+02	0.50835D+02	
Energy	0.29613D+03	0.29327D+03	kJ/mol
Enthalpy	0.29861D+03	0.29575D+03	kJ/mol
Entropy	0.34105D+03	0.34938D+03	J/(mol K)
Sp.Heat(V)	0.10088D+03	0.10334D+03	J/(mol K)
Sp.Heat(P)	0.10920D+03	0.11165D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.57811D-47	0.49820D-46	
QZvib	0.26477D+02	0.50835D+02	
Energy	0.29613D+03	0.29327D+03	kJ/mol
Enthalpy	0.29861D+03	0.29575D+03	kJ/mol
Entropy	0.34105D+03	0.34938D+03	J/(mol K)
Sp.Heat(V)	0.10088D+03	0.10334D+03	J/(mol K)
Sp.Heat(P)	0.10920D+03	0.11165D+03	J/(mol K)

5a-4 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.195843503

Zero-point correction= 0.105014 (Hartree/Particle)
Thermal correction to Energy= 0.111005
Thermal correction to Enthalpy= 0.111949
Thermal correction to Gibbs Free Energy= 0.075408
Sum of electronic and ZPE= -604.090830
Sum of electronic and thermal Energies= -604.084839
Sum of electronic and thermal Enthalpies= -604.083895
Sum of electronic and thermal Free Energies= -604.120436

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.656	21.542	76.907

C,0,-0.1171214429,-0.126979629,-0.2152716036
C,0,-0.2028462709,-0.2291805562,1.2831373936
H,0,-0.8163165246,1.3773030586,1.6735063638
B,0,0.2930878548,1.3421885275,2.2128149628
C,0,0.9206872531,-0.2690195486,2.1329404777
H,0,-1.0117540889,0.3312412221,-0.6448510891
H,0,-0.0270188837,-1.1445939159,-0.6148883731

H,0,-1.1472405118,-0.5973486551,1.6788300398
H,0,1.9108986785,-0.234868338,1.6890492195
H,0,0.8460640401,-0.7744262097,3.089008476
H,0,0.0372822326,1.5356797315,3.3629958087
Cl,0,1.39146441,2.559256314,1.3517759562
H,0,0.7601932537,0.4440179988,-0.5260776324

B3LYP/6-31G*
E(RB+HF-LYP) = -604.174764899

Zero-point correction= 0.104948 (Hartree/Particle)
Thermal correction to Energy= 0.110261
Thermal correction to Enthalpy= 0.111205
Thermal correction to Gibbs Free Energy= 0.075869
Sum of electronic and ZPE= -604.069817
Sum of electronic and thermal Energies= -604.064504
Sum of electronic and thermal Enthalpies= -604.063560
Sum of electronic and thermal Free Energies= -604.098896

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.190	19.341	74.370

C,0,-0.0900580815,-0.1431287104,-0.2069286872
C,0,-0.1553299851,-0.2046983284,1.3155566411
H,0,-0.8449333814,1.0866158175,1.6425958065
B,0,0.2470138334,1.3780775467,2.2744963573
C,0,1.0403132793,-0.1844052322,2.132998153
H,0,-0.3101907747,0.8569587512,-0.5898126959
H,0,-0.8125089909,-0.8412917987,-0.6401252506
H,0,-1.0063737495,-0.7517207086,1.721895689
H,0,1.9930185231,-0.1153334881,1.6169662591
H,0,1.0415450898,-0.7562422444,3.054931707
H,0,-0.200168098,1.5588999432,3.3640858533
Cl,0,1.0261594782,2.7452198167,1.343048898
H,0,0.9088928574,-0.4156813646,-0.5567387306

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101511	E(Thermal)=	0.107614
E(QCISD(T))=	-603.097405	(Empiric)=	-0.101400
DE(Plus)=	-0.009491	DE(2DF)=	-0.209397
E(Delta-G3)=	-0.560989	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.877172	G3 Energy=	-603.871069
G3 Enthalpy=	-603.870125	G3 Free Energy=	-603.906845

For Anharmonic Corrections of 5a-4

Zero-point vibrational energy 277584.0 (Joules/Mol)
66.34416 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 197.96 252.50 403.74 547.73 623.30
(Kelvin) 748.64 924.83 1022.83 1246.64 1319.22
1345.51 1380.36 1453.56 1489.89 1543.86
1616.09 1721.55 1784.99 1872.52 2050.26
2098.14 2165.97 2191.23 2241.36 3422.50
3801.36 4407.06 4506.55 4553.27 4565.26
4580.90 4691.68

Zero-point correction= 0.105726 (Hartree/Particle)
Thermal correction to Energy= 0.111720
Thermal correction to Enthalpy= 0.112664
Thermal correction to Gibbs Free Energy= 0.076085
Sum of electronic and zero-point Energies= -604.073315
Sum of electronic and thermal Energies= -604.067321
Sum of electronic and thermal Enthalpies= -604.066376
Sum of electronic and thermal Free Energies= -604.102956

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.105	21.424	76.988

ZPE(harm) = 0.27493D+03 kJ/mol ZPE(anh)= 0.27084D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.57652D-47	0.30381D-46	
QZvib	0.84564D+01	0.85284D+01	
Energy	0.29067D+03	0.28674D+03	kJ/mol
Enthalpy	0.29315D+03	0.28922D+03	kJ/mol
Entropy	0.33043D+03	0.33106D+03	J/(mol K)
Sp.Heat(V)	0.89637D+02	0.91349D+02	J/(mol K)
Sp.Heat(P)	0.97951D+02	0.99663D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value
Qvib	0.57652D-47	0.30381D-46
QZvib	0.84564D+01	0.85284D+01

Energy	0.29067D+03	0.28674D+03	kJ/mol
Enthalpy	0.29315D+03	0.28922D+03	kJ/mol
Entropy	0.33043D+03	0.33106D+03	J/(mol K)
Sp.Heat(V)	0.89637D+02	0.91349D+02	J/(mol K)
Sp.Heat(P)	0.97951D+02	0.99663D+02	J/(mol K)

5a-6 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.196191233

Zero-point correction= 0.104966 (Hartree/Particle)
Thermal correction to Energy= 0.111025
Thermal correction to Enthalpy= 0.111969
Thermal correction to Gibbs Free Energy= 0.075270
Sum of electronic and ZPE= -604.091225
Sum of electronic and thermal Energies= -604.085167
Sum of electronic and thermal Enthalpies= -604.084223
Sum of electronic and thermal Free Energies= -604.120921

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.669	21.564	77.239

C,0,-0.155887754,-0.1517483725,-0.2174675163
C,0,-0.1885733195,-0.1886864244,1.2887605106
C,0,0.9774101069,-0.2437860183,2.076786595
B,0,0.3096242945,1.3413571848,2.2558426106
H,0,1.1671056468,2.0929529679,1.8979234047
H,0,-0.5761178498,1.5118567464,1.4169485926
H,0,-1.0539674873,0.3055845982,-0.640572216
H,0,-0.0925009633,-1.1854360934,-0.5793837567
H,0,-1.1244258866,-0.5009941507,1.7469950667
H,0,1.9431712615,-0.2376423635,1.581147368
H,0,0.9417925082,-0.7251044256,3.0476721912
Cl,0,-0.445319979,1.5793708052,3.928281355
H,0,0.7241394218,0.3853455458,-0.5813342055

B3LYP/6-31G*
E(RB+HF-LYP) = -604.174187665

Zero-point correction= 0.104872 (Hartree/Particle)
Thermal correction to Energy= 0.110312

Thermal correction to Enthalpy= 0.111256
Thermal correction to Gibbs Free Energy= 0.075662
Sum of electronic and ZPE= -604.069316
Sum of electronic and thermal Energies= -604.063875
Sum of electronic and thermal Enthalpies= -604.062931
Sum of electronic and thermal Free Energies= -604.098525

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.222	19.453	74.915

C,0,-0.1181286712,-0.1620936418,-0.2188607924
C,0,-0.1388966993,-0.1718672021,1.3096302124
C,0,1.0859247377,-0.1422483715,2.0777324716
B,0,0.2415971067,1.3800553705,2.3234928102
H,0,0.7915076497,2.2915084668,1.7862651986
H,0,-0.7409879505,1.1875332026,1.5084193487
H,0,-0.3502686564,0.8210135579,-0.6379315599
H,0,-0.855370238,-0.8713544572,-0.6072182103
H,0,-0.979556702,-0.6913448855,1.7675747608
H,0,2.0189385542,-0.0516147671,1.5298773683
H,0,1.1275470291,-0.7203539618,2.9949795515
Cl,0,-0.5252000674,1.570188702,3.9726885368
H,0,0.8693439074,-0.4563520129,-0.5850496964

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101409	E(Thermal)=	0.107602
E(QCISD(T))=	-603.097399	E(Empiric)=	-0.101400
DE(Plus)=	-0.009976	DE(2DF)=	-0.209260
E(Delta-G3)=	-0.560487	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.877112	G3 Energy=	-603.870919
G3 Enthalpy=	-603.869975	G3 Free Energy=	-603.906921

5a-7 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.189970198

Zero-point correction= 0.105086 (Hartree/Particle)
Thermal correction to Energy= 0.111131
Thermal correction to Enthalpy= 0.112075
Thermal correction to Gibbs Free Energy= 0.075436

Sum of electronic and ZPE= -604.084884
Sum of electronic and thermal Energies= -604.078840
Sum of electronic and thermal Enthalpies= -604.077895
Sum of electronic and thermal Free Energies= -604.114534

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.736	21.504	77.114

C,0,-0.1341176462,0.1705630807,1.0637333044
B,0,0.4742458471,1.6672790931,1.9182021664
C,0,1.1025168762,0.0485120329,1.7352452714
C,0,2.4272406141,-0.0666397955,1.005304729
H,0,-0.1563746688,0.3675846313,-0.0050406004
H,0,-1.0467996021,-0.2440559046,1.4809880936
H,0,1.0705165493,-0.4462996535,2.7024061201
H,0,0.3701729593,1.8270165697,3.0953387033
H,0,-0.7104849604,1.6838558011,1.5579869663
Cl,0,1.37281314,2.94322584,0.9347237727
H,0,3.230353124,0.4202170505,1.5656994523
H,0,2.6878292782,-1.1250614227,0.8870816017
H,0,2.3890684895,0.392062677,0.0151504192

B3LYP/6-31G*
E(RB+HF-LYP) = -604.170085482

Zero-point correction= 0.105533 (Hartree/Particle)
Thermal correction to Energy= 0.110876
Thermal correction to Enthalpy= 0.111820
Thermal correction to Gibbs Free Energy= 0.076530
Sum of electronic and ZPE= -604.064553
Sum of electronic and thermal Energies= -604.059209
Sum of electronic and thermal Enthalpies= -604.058265
Sum of electronic and thermal Free Energies= -604.093555

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.576	19.327	74.274

C,0,-0.1393622666,0.2848307405,0.9855206268
B,0,0.5113887389,1.622177126,2.0465092008
C,0,1.0716957669,0.0212515853,1.6710921941
C,0,2.415260151,-0.1003395553,0.9573057816
H,0,-0.1171494723,0.6110257177,-0.0516844475

H,0,-1.0810438701,-0.1446519812,1.3170783668
H,0,0.9697156915,-0.5917504779,2.5621549984
H,0,0.351392473,1.6482726403,3.2289214073
H,0,-0.663888082,1.7364379077,1.6469612393
Cl,0,1.4659423465,2.9833706044,1.2542368387
H,0,2.9273125341,0.8608737931,0.8620514427
H,0,3.0656321004,-0.7726097603,1.5245081802
H,0,2.3000838888,-0.5206283404,-0.0478358293

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101571	E(Thermal)=	0.107749
E(QCISD(T))=	-603.092213	E(Empiric)=	-0.101400
DE(Plus)=	-0.009551	DE(2DF)=	-0.209658
E(Delta-G3)=	-0.560704	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.871955	G3 Energy=	-603.865777
G3 Enthalpy=	-603.864833	G3 Free Energy=	-603.901714

For Anharmonic Corrections of 5a-7

Zero-point vibrational energy 277675.2 (Joules/Mol)
66.36597 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 177.49 289.83 298.38 525.26 611.42
(Kelvin) 819.31 897.47 1060.80 1207.44 1285.55
1353.78 1438.26 1487.29 1557.95 1580.98
1617.81 1742.04 1756.59 1882.63 2064.04
2094.73 2175.90 2189.40 2225.11 3366.88
3823.96 4407.00 4501.55 4542.58 4553.50
4577.29 4680.98

Zero-point correction=	0.105761 (Hartree/Particle)
Thermal correction to Energy=	0.111827
Thermal correction to Enthalpy=	0.112771
Thermal correction to Gibbs Free Energy=	0.076004
Sum of electronic and zero-point Energies=	-604.067441
Sum of electronic and thermal Energies=	-604.061375
Sum of electronic and thermal Enthalpies=	-604.060430
Sum of electronic and thermal Free Energies=	-604.097198

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.173	21.380	77.384

ZPE(harm) = 0.27403D+03 kJ/mol ZPE(anh)= 0.27089D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.96767D-47	0.19823D-46	
QZvib	0.98718D+01	0.56950D+01	
Energy	0.28996D+03	0.28622D+03	kJ/mol
Enthalpy	0.29244D+03	0.28870D+03	kJ/mol
Entropy	0.33209D+03	0.32551D+03	J/(mol K)
Sp.Heat(V)	0.89455D+02	0.89872D+02	J/(mol K)
Sp.Heat(P)	0.97769D+02	0.98186D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.96767D-47	0.19823D-46	
QZvib	0.98718D+01	0.56950D+01	
Energy	0.28996D+03	0.28622D+03	kJ/mol
Enthalpy	0.29244D+03	0.28870D+03	kJ/mol
Entropy	0.33209D+03	0.32551D+03	J/(mol K)
Sp.Heat(V)	0.89455D+02	0.89872D+02	J/(mol K)
Sp.Heat(P)	0.97769D+02	0.98186D+02	J/(mol K)

5a-8 Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -604.191792527

Zero-point correction= 0.104955 (Hartree/Particle)
Thermal correction to Energy= 0.110976
Thermal correction to Enthalpy= 0.111920
Thermal correction to Gibbs Free Energy= 0.075318
Sum of electronic and ZPE= -604.086838
Sum of electronic and thermal Energies= -604.080816
Sum of electronic and thermal Enthalpies= -604.079872
Sum of electronic and thermal Free Energies= -604.116475

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.639	21.486	77.037

C,0,0.014602279,0.0522443927,1.1343095034
C,0,1.2581411843,0.0836186148,1.8057019364
C,0,2.5733935066,0.0261680609,1.0537102503
B,0,0.4822523131,1.6193088168,1.9375972643
H,0,1.258070667,2.4026261825,1.484100863
H,0,-0.027341366,0.0605705628,0.0477449787

H,0,-0.8796552581,-0.3053435861,1.6348395299
H,0,1.2669709244,-0.3245734792,2.8132235945
Cl,0,-0.2338470739,1.9311019899,3.6109242202
H,0,-0.4354008535,1.6789556551,1.1021073727
H,0,3.3658417834,0.5332211762,1.6115596837
H,0,2.8826397501,-1.0145239096,0.8973516723
H,0,2.4960321435,0.505845523,0.0727891307

B3LYP/6-31G*
E(RB+HF-LYP) = -604.171231333

Zero-point correction= 0.105440 (Hartree/Particle)
Thermal correction to Energy= 0.110872
Thermal correction to Enthalpy= 0.111816
Thermal correction to Gibbs Free Energy= 0.076272
Sum of electronic and ZPE= -604.065791
Sum of electronic and thermal Energies= -604.060359
Sum of electronic and thermal Enthalpies= -604.059415
Sum of electronic and thermal Free Energies= -604.094960

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.573	19.502	74.810

C,0,0.0078793466,0.1708255377,1.0478677155
C,0,1.224428836,0.0348972808,1.7359335316
C,0,2.5625568507,-0.0145527448,1.0064993821
B,0,0.4966362295,1.6006693076,2.0625364618
H,0,1.3689289343,2.3670559079,1.7944445915
H,0,-0.0002978293,0.3236567338,-0.0293103617
H,0,-0.9253571831,-0.1778548311,1.4791403015
H,0,1.1782734602,-0.4692052188,2.6968085554
Cl,0,-0.2749956545,1.6801129851,3.737288136
H,0,-0.3579448572,1.8510802392,1.2090387922
H,0,3.0170851784,0.9731494113,0.8935826348
H,0,3.2672445322,-0.6379320348,1.565153117
H,0,2.4572621563,-0.4526825739,0.0069771423

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101431	E(Thermal)=	0.107597
E(QCISD(T))=	-603.093719	E(Empiric)=	-0.101400
DE(Plus)=	-0.009713	DE(2DF)=	-0.209351
E(Delta-G3)=	-0.560409	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.873162	G3 Energy=	-603.866997

G3 Enthalpy= -603.866052 G3 Free Energy= -603.902920

For Anharmonic Corrections of 5a-8

Zero-point vibrational energy 277732.4 (Joules/Mol)
66.37963 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 206.77 279.40 366.60 430.61 605.81
(Kelvin) 809.63 926.43 1031.98 1233.93 1280.67
1355.14 1420.63 1472.18 1558.37 1566.96
1613.30 1722.59 1759.72 1869.70 2060.29
2099.07 2179.42 2195.52 2245.78 3460.46
3825.15 4393.16 4484.21 4516.97 4557.08
4589.54 4689.90

Zero-point correction= 0.105783 (Hartree/Particle)
Thermal correction to Energy= 0.111837
Thermal correction to Enthalpy= 0.112781
Thermal correction to Gibbs Free Energy= 0.076082
Sum of electronic and zero-point Energies= -604.069254
Sum of electronic and thermal Energies= -604.063200
Sum of electronic and thermal Enthalpies= -604.062256
Sum of electronic and thermal Free Energies= -604.098955

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.179	21.462	77.240

ZPE(harm) = 0.27464D+03 kJ/mol ZPE(anh)= 0.27053D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.67487D-47	0.44140D-46	
QZvib	0.87965D+01	0.10948D+02	
Energy	0.29054D+03	0.28684D+03	kJ/mol
Enthalpy	0.29302D+03	0.28932D+03	kJ/mol
Entropy	0.33149D+03	0.33469D+03	J/(mol K)
Sp.Heat(V)	0.89797D+02	0.91680D+02	J/(mol K)
Sp.Heat(P)	0.98111D+02	0.99994D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value

Qvib	0.67487D-47	0.44140D-46	
QZvib	0.87965D+01	0.10948D+02	
Energy	0.29054D+03	0.28684D+03	kJ/mol
Enthalpy	0.29302D+03	0.28932D+03	kJ/mol
Entropy	0.33149D+03	0.33469D+03	J/(mol K)
Sp.Heat(V)	0.89797D+02	0.91680D+02	J/(mol K)
Sp.Heat(P)	0.98111D+02	0.99994D+02	J/(mol K)

5a-9 Variational Transition State

B3LYP/6-31G**
E(RB+HF-LYP) = -604.197470310

Zero-point correction= 0.101807 (Hartree/Particle)
Thermal correction to Energy= 0.109894
Thermal correction to Enthalpy= 0.110838
Thermal correction to Gibbs Free Energy= 0.065892
Sum of electronic and zero-point Energies= -604.095663
Sum of electronic and thermal Energies= -604.087576
Sum of electronic and thermal Enthalpies= -604.086632
Sum of electronic and thermal Free Energies= -604.131578

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.959	24.380	94.596

B3LYP/6-31G*
E(RB+HF-LYP) = -604.179520482

Zero-point correction= 0.102447 (Hartree/Particle)
Thermal correction to Energy= 0.110537
Thermal correction to Enthalpy= 0.111481
Thermal correction to Gibbs Free Energy= 0.066307
Sum of electronic and ZPE= -604.077074
Sum of electronic and thermal Energies= -604.068983
Sum of electronic and thermal Enthalpies= -604.068039
Sum of electronic and thermal Free Energies= -604.113214

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	69.363	24.319	95.079

C,0,-1.38084,0.96215,-0.58515

C,0,-1.85043,0.12939,0.3481
C,0,-2.31457,-1.27712,0.10082
B,0,1.75881,0.5343,0.74275
Cl,0,2.86804,-0.28422,-0.34834
H,0,-1.29654,0.66161,-1.6279
H,0,-1.08131,1.97879,-0.34646
H,0,-1.92422,0.48223,1.37778
H,0,1.26518,-0.10245,1.61625
H,0,1.59643,1.70246,0.59686
H,0,-1.74685,-1.99524,0.70714
H,0,-3.3701,-1.39646,0.38014
H,0,-2.20643,-1.55783,-0.95201

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.098349	E(Thermal)=	0.106584
E(QCISD(T))=	-603.098660	E(Empiric)=	-0.101400
DE(Plus)=	-0.010343	DE(2DF)=	-0.204867
E(Delta-G3)=	-0.561452	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.878373	G3 Energy=	-603.870137
G3 Enthalpy=	-603.869193	G3 Free Energy=	-603.914731

5a-10 Variational Transition State
B3LYP/6-31G**
E(RB+HF-LYP) = -604.197880729

Zero-point correction= 0.101957 (Hartree/Particle)
Thermal correction to Energy= 0.109908
Thermal correction to Enthalpy= 0.110852
Thermal correction to Gibbs Free Energy= 0.067117
Sum of electronic and zero-point Energies= -604.095924
Sum of electronic and thermal Energies= -604.087973
Sum of electronic and thermal Enthalpies= -604.087029
Sum of electronic and thermal Free Energies= -604.130764

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.968	24.315	92.048

B3LYP/6-31G*
E(RB+HF-LYP) = -604.180096766

Zero-point correction= 0.102579 (Hartree/Particle)

Thermal correction to Energy= 0.110548
Thermal correction to Enthalpy= 0.111493
Thermal correction to Gibbs Free Energy= 0.067508
Sum of electronic and ZPE= -604.077518
Sum of electronic and thermal Energies= -604.069548
Sum of electronic and thermal Enthalpies= -604.068604
Sum of electronic and thermal Free Energies= -604.112589

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.370	24.255	92.574

C,0,-2.39506,-1.08008,0.08618
C,0,-1.56542,0.00394,-0.53927
C,0,-1.17519,1.1272,0.07122
B,0,1.69448,-0.21122,0.83335
Cl,0,2.91866,0.00044,-0.41507
H,0,1.50956,0.68822,1.58754
H,0,1.16266,-1.27048,0.91632
H,0,-1.86886,-2.04356,0.06484
H,0,-3.33351,-1.22291,-0.46621
H,0,-1.2798,-0.15429,-1.58024
H,0,-1.44308,1.33717,1.10471
H,0,-0.5942,1.88722,-0.44466
H,0,-2.64325,-0.84859,1.1272

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.098476	E(Thermal)=	0.106594
E(QCISD(T))=	-603.099329	E(Empiric)=	-0.101400
DE(Plus)=	-0.010367	DE(2DF)=	-0.205034
E(Delta-G3)=	-0.561331	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.878986	G3 Energy=	-603.870868
G3 Enthalpy=	-603.869924	G3 Free Energy=	-603.914270

5a-11 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.245449163
Zero-point correction= 0.107202 (Hartree/Particle)
Thermal correction to Energy= 0.114005
Thermal correction to Enthalpy= 0.114949
Thermal correction to Gibbs Free Energy= 0.075908
Sum of electronic and ZPE= -604.138247

Sum of electronic and thermal Energies= -604.131445
Sum of electronic and thermal Enthalpies= -604.130500
Sum of electronic and thermal Free Energies= -604.169541

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	72.005	22.553	82.140

C,0,-0.188149372,-0.5819119493,-0.3099271957
C,0,-0.2985920645,0.4942445974,0.7762588335
C,0,0.6603619392,0.2630788033,1.9532347728
B,0,0.6857751248,1.2600403442,3.1514735225
H,0,1.4172213297,1.1096544269,4.0807453937
Cl,0,-0.3583526062,2.6887972782,3.2370311694
H,0,-0.1036045929,1.4802664865,0.3365903478
H,0,-0.8832908108,-0.3897357552,-1.1344360749
H,0,-0.4154013709,-1.5766469187,0.0922468529
H,0,-1.3294592482,0.5339912965,1.1495082507
H,0,1.703222915,0.1982611232,1.5933122078
H,0,0.4933133363,-0.7357078147,2.3956942609
H,0,0.8243194203,-0.6196289181,-0.7298953412

B3LYP/6-31G*
E(RB+HF-LYP) = -604.228936025

Zero-point correction= 0.107965 (Hartree/Particle)
Thermal correction to Energy= 0.114750
Thermal correction to Enthalpy= 0.115694
Thermal correction to Gibbs Free Energy= 0.076650
Sum of electronic and ZPE= -604.120971
Sum of electronic and thermal Energies= -604.114186
Sum of electronic and thermal Enthalpies= -604.113242
Sum of electronic and thermal Free Energies= -604.152286

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	72.007	22.557	82.175

C,0,-0.1877981702,-0.5807046296,-0.3088316453
C,0,-0.2979367701,0.4942596862,0.7771724875
C,0,0.661724574,0.2608509202,1.9529540339
B,0,0.6841601197,1.2606282509,3.1506016852
H,0,1.4156569835,1.1113328679,4.0814220797
Cl,0,-0.361348137,2.6876200448,3.2324991373

H,0,-0.102626516,1.4813124075,0.3388803484
H,0,-0.8834357604,-0.3878131961,-1.1334841074
H,0,-0.4149809991,-1.5762130615,0.0928905876
H,0,-1.328779572,0.5345410565,1.1517027936
H,0,1.7042275246,0.1961851685,1.5912605035
H,0,0.4934312887,-0.7386303158,2.3939474015
H,0,0.8250694343,-0.6186661995,-0.7291783055

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.103646	E(Thermal)=	0.110596
E(QCISD(T))=	-603.148892	E(Empiric)=	-0.101400
DE(Plus)=	-0.008884	DE(2DF)=	-0.207569
E(Delta-G3)=	-0.561291	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.924390	G3 Energy=	-603.917440
G3 Enthalpy=	-603.916496	G3 Free Energy=	-603.955869

5a-12 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.244920071

Zero-point correction= 0.106898 (Hartree/Particle)
Thermal correction to Energy= 0.113026
Thermal correction to Enthalpy= 0.113970
Thermal correction to Gibbs Free Energy= 0.076786
Sum of electronic and ZPE= -604.138022
Sum of electronic and thermal Energies= -604.131894
Sum of electronic and thermal Enthalpies= -604.130950
Sum of electronic and thermal Free Energies= -604.168135

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.925	20.935	78.262

C,0,-0.3652539027,-0.6630935398,-0.2136089526
C,0,-0.4832315724,0.249514819,1.0121157964
H,0,-0.9550392299,1.19572399,0.7163051489
B,0,0.8291776936,1.4378335858,2.9607445328
C,0,0.8716770559,0.5429642339,1.6823722945
H,0,-1.3439100826,-0.8524223478,-0.6679607102
H,0,0.0712691575,-1.6324620356,0.055631824
H,0,-1.1599470346,-0.2071195976,1.745979301
H,0,1.5792240974,0.9756196664,0.9578171248
H,0,1.3534175546,-0.4050970274,1.982785779

H,0,-0.1702195054,1.7612048121,3.5251298877
Cl,0,2.3328236435,2.0243959073,3.6957599676
H,0,0.2773921252,-0.2137924663,-0.9801019939

B3LYP/6-31G*
E(RB+HF-LYP) = -604.228389629

Zero-point correction= 0.107820 (Hartree/Particle)
Thermal correction to Energy= 0.114765
Thermal correction to Enthalpy= 0.115710
Thermal correction to Gibbs Free Energy= 0.076050
Sum of electronic and ZPE= -604.120570
Sum of electronic and thermal Energies= -604.113624
Sum of electronic and thermal Enthalpies= -604.112680
Sum of electronic and thermal Free Energies= -604.152339

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	72.016	22.708	83.470

C,0,-0.1738849443,-0.5467620613,-0.2984003938
C,0,-0.3582712752,0.4583070348,0.8428128041
C,0,0.6597278005,0.2683405896,1.9850878547
B,0,0.6121087131,1.3419713263,3.117294416
H,0,0.2410492229,2.4633283806,2.9460184353
H,0,-0.2785760373,1.4807125094,0.4504020883
H,0,-0.9171281583,-0.3945223535,-1.0894024572
H,0,-0.2756667182,-1.5779846263,0.0614445396
H,0,-1.3765171891,0.3681776944,1.2446492395
H,0,1.6823170273,0.3508570212,1.5671722536
H,0,0.608737859,-0.7510171487,2.3915675633
Cl,0,1.1815213781,0.9738622341,4.7540721594
H,0,0.8210323213,-0.4522006005,-0.7511185026

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.103507	E(Thermal)=	0.110613
E(QCISD(T))=	-603.148158	E(Empiric)=	-0.101400
DE(Plus)=	-0.008766	DE(2DF)=	-0.207245
E(Delta-G3)=	-0.561250	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.923313	G3 Energy=	-603.916206
G3 Enthalpy=	-603.915262	G3 Free Energy=	-603.955253

For Anharmonic Corrections of 5a-12

Zero-point vibrational energy 276176.1 (Joules/Mol)
66.00768 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 218.65 314.51 363.22 418.46 620.34
(Kelvin) 890.16 908.98 1051.05 1247.29 1300.87
1360.32 1384.26 1447.97 1486.26 1556.84
1607.74 1739.84 1793.18 1880.39 2023.01
2076.14 2166.19 2186.29 2192.37 3097.52
3849.96 4407.66 4505.78 4529.16 4558.57
4560.71 4688.91

Zero-point correction= 0.105190 (Hartree/Particle)
Thermal correction to Energy= 0.111173
Thermal correction to Enthalpy= 0.112117
Thermal correction to Gibbs Free Energy= 0.075586
Sum of electronic and zero-point Energies= -604.073853
Sum of electronic and thermal Energies= -604.067869
Sum of electronic and thermal Enthalpies= -604.066925
Sum of electronic and thermal Free Energies= -604.103456

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.762	21.368	76.886

ZPE(harm) = 0.27175D+03 kJ/mol ZPE(anh)= 0.26752D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.19363D-46	0.14136D-45	
QZvib	0.78705D+01	0.10432D+02	
Energy	0.28746D+03	0.28375D+03	kJ/mol
Enthalpy	0.28994D+03	0.28623D+03	kJ/mol
Entropy	0.33001D+03	0.33409D+03	J/(mol K)
Sp.Heat(V)	0.89404D+02	0.91487D+02	J/(mol K)
Sp.Heat(P)	0.97719D+02	0.99801D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.19363D-46	0.14136D-45	
QZvib	0.78705D+01	0.10432D+02	
Energy	0.28746D+03	0.28375D+03	kJ/mol
Enthalpy	0.28994D+03	0.28623D+03	kJ/mol
Entropy	0.33001D+03	0.33409D+03	J/(mol K)

Sp.Heat(V)	0.89404D+02	0.91487D+02	J/(mol K)
Sp.Heat(P)	0.97719D+02	0.99801D+02	J/(mol K)

5a-13 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.242349463

Zero-point correction= 0.107124 (Hartree/Particle)
Thermal correction to Energy= 0.113984
Thermal correction to Enthalpy= 0.114928
Thermal correction to Gibbs Free Energy= 0.075782
Sum of electronic and ZPE= -604.135225
Sum of electronic and thermal Energies= -604.128366
Sum of electronic and thermal Enthalpies= -604.127422
Sum of electronic and thermal Free Energies= -604.166567

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	71.526	23.153	82.388

C,0,0.1187566042,-0.2314700389,-0.133763511
C,0,-0.1344826102,0.3010303902,1.2852853019
H,0,-0.2619612452,2.350325165,2.5574384313
B,0,-0.1584743097,1.8550258369,1.4774715202
C,0,0.804462041,-0.3626550375,2.3236953824
H,0,-0.5848561384,0.1888137276,-0.8587534832
H,0,0.0242196744,-1.3232259726,-0.1648637531
H,0,-1.1657390888,0.0194984073,1.5795995704
H,0,1.8540801753,-0.1297127137,2.1088476254
H,0,0.6999959668,-1.4533389686,2.2983631909
H,0,0.5899212894,-0.0261510241,3.3433305058
Cl,0,-0.0775735663,3.0021989438,0.1308461181
H,0,1.1290312075,0.0229312845,-0.4745268993

B3LYP/6-31G*
E(RB+HF-LYP) = -604.226104485

Zero-point correction= 0.107953 (Hartree/Particle)
Thermal correction to Energy= 0.114791
Thermal correction to Enthalpy= 0.115735
Thermal correction to Gibbs Free Energy= 0.076501
Sum of electronic and ZPE= -604.118151
Sum of electronic and thermal Energies= -604.111314

Sum of electronic and thermal Enthalpies= -604.110370
Sum of electronic and thermal Free Energies= -604.149603

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	72.032	22.983	82.574

C,0,0.1120407443,-0.2468615743,-0.1279614326
C,0,-0.1499082495,0.301555544,1.2822965388
H,0,-0.325702872,2.3659588921,2.5246307865
B,0,-0.1475692836,1.8585906876,1.4589129432
C,0,0.7877508599,-0.3487956511,2.3314441609
H,0,-0.5852017333,0.1701722676,-0.8620537192
H,0,0.0122645178,-1.3390045329,-0.149231641
H,0,-1.1800127892,0.021969945,1.5782411539
H,0,1.8385699461,-0.1187036248,2.1173018216
H,0,0.6824397652,-1.4401624716,2.3177032771
H,0,0.56999892,-0.0007692003,3.3471418083
Cl,0,0.0968264551,2.9894568738,0.1192340161
H,0,1.1258837192,-0.0001371552,-0.4646897136

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.103635	E(Thermal)=	0.110643
E(QCISD(T))=	-603.147123	E(Empiric)=	-0.101400
DE(Plus)=	-0.009167	DE(2DF)=	-0.208033
E(Delta-G3)=	-0.560837	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.922925	G3 Energy=	-603.915917
G3 Enthalpy=	-603.914973	G3 Free Energy=	-603.954544

Propene
B3LYP/6-31+G**
E(RB+HF-LYP) = -117.922799177

Zero-point correction= 0.079556 (Hartree/Particle)
Thermal correction to Energy= 0.083653
Thermal correction to Enthalpy= 0.084597
Thermal correction to Gibbs Free Energy= 0.054531
Sum of electronic and ZPE= -117.843243
Sum of electronic and thermal Energies= -117.839146
Sum of electronic and thermal Enthalpies= -117.838202
Sum of electronic and thermal Free Energies= -117.868268

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 52.493 13.015 63.280

C,0,0.0344608581,-0.1196186007,-0.0253367535
H,0,-0.7225196876,0.6145938205,-0.3292384394
C,0,0.0641536597,-0.2773363759,1.4684961103
C,0,1.1264931839,-0.0522279939,2.2475837269
H,0,-0.229463632,-1.0649677664,-0.5163525082
H,0,-0.8672370321,-0.6026054777,1.9338697675
H,0,2.0784454947,0.2734473875,1.833158635
H,0,1.0819141746,-0.1852657575,3.324646825
H,0,1.0037429807,0.2082407643,-0.4141473637

propene_G3B3_G8_med
sm_clanti
B3LYP/6-31G*
E(RB+HF-LYP) = -117.907556179

Zero-point correction= 0.080081 (Hartree/Particle)
Thermal correction to Energy= 0.084158
Thermal correction to Enthalpy= 0.085102
Thermal correction to Gibbs Free Energy= 0.055079
Sum of electronic and ZPE= -117.827475
Sum of electronic and thermal Energies= -117.823398
Sum of electronic and thermal Enthalpies= -117.822454
Sum of electronic and thermal Free Energies= -117.852477

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 52.810 12.917 63.189

C,0,0.0345565707,-0.1197608226,-0.0234351422
H,0,-0.7220376636,0.6151139371,-0.330185343
C,0,0.0640978356,-0.277641459,1.4700545078
C,0,1.1246474375,-0.0526175058,2.2461570925
H,0,-0.2287854144,-1.0648944572,-0.5174128732
H,0,-0.8686000739,-0.6030047319,1.9335519938
H,0,2.0769329525,0.2730371984,1.8315449994
H,0,1.084559352,-0.1842527935,3.3241654131
H,0,1.0046190036,0.2082806345,-0.4117606481

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.076878 E(Thermal)= 0.081041

E(QCISD(T))=	-117.508195	E(Empiric)=	-0.060840
DE(Plus)=	-0.007429	DE(2DF)=	-0.116313
E(Delta-G3)=	-0.168940	E(G3-Empiric)=	-0.060840
G3(0 K)=	-117.784839	G3 Energy=	-117.780675
G3 Enthalpy=	-117.779731	G3 Free Energy=	-117.809894

For Anharmonic Corrections Of Propene

Zero-point vibrational energy 210198.2 (Joules/Mol)
50.23857 (Kcal/Mol)
Warning -- explicit consideration of 3 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 289.91 609.04 843.87 1339.89 1340.38
(Kelvin) 1372.37 1485.77 1554.10 1730.75 1922.49
2060.80 2115.88 2170.59 2190.64 2484.78
4373.25 4443.46 4492.28 4530.66 4546.95
4664.16

Zero-point correction= 0.080060 (Hartree/Particle)
Thermal correction to Energy= 0.084155
Thermal correction to Enthalpy= 0.085099
Thermal correction to Gibbs Free Energy= 0.055030
Sum of electronic and zero-point Energies= -117.827479
Sum of electronic and thermal Energies= -117.823384
Sum of electronic and thermal Enthalpies= -117.822440
Sum of electronic and thermal Free Energies= -117.852509

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	52.808	12.955	63.285

ZPE(harm) = 0.21020D+03 kJ/mol ZPE(anh)= 0.20739D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.30971D-36	0.10555D-35	
QZvib	0.20703D+01	0.22735D+01	
Energy	0.22095D+03	0.21831D+03	kJ/mol
Enthalpy	0.22343D+03	0.22079D+03	kJ/mol
Entropy	0.26478D+03	0.26612D+03	J/(mol K)
Sp.Heat(V)	0.54204D+02	0.55064D+02	J/(mol K)
Sp.Heat(P)	0.62518D+02	0.63378D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.30971D-36	0.10555D-35	
QZvib	0.20703D+01	0.22735D+01	
Energy	0.22095D+03	0.21831D+03	kJ/mol
Enthalpy	0.22343D+03	0.22079D+03	kJ/mol
Entropy	0.26478D+03	0.26612D+03	J/(mol K)
Sp.Heat(V)	0.54204D+02	0.55064D+02	J/(mol K)
Sp.Heat(P)	0.62518D+02	0.63378D+02	J/(mol K)

5b-1 Starting Material
B3LYP/6-31+G**
E(RB+HF-LYP) = -945.924297177

Zero-point correction= 0.014886 (Hartree/Particle)
Thermal correction to Energy= 0.018411
Thermal correction to Enthalpy= 0.019355
Thermal correction to Gibbs Free Energy= -0.011723
Sum of electronic and ZPE= -945.909411
Sum of electronic and thermal Energies= -945.905887
Sum of electronic and thermal Enthalpies= -945.904942
Sum of electronic and thermal Free Energies= -945.936020

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	11.603	9.859	65.396

B,0,0.1276529986,2.3051483904,2.3633551164
Cl,0,1.4739014992,3.0846499732,1.5610229442
Cl,0,-1.2481013032,1.7169757157,1.4556989428
H,0,0.1493228054,2.1725099208,3.5407849967

B3LYP/6-31G*
E(RB+HF-LYP) = -945.920195673

Zero-point correction= 0.014969 (Hartree/Particle)
Thermal correction to Energy= 0.018490
Thermal correction to Enthalpy= 0.019434
Thermal correction to Gibbs Free Energy= -0.011638
Sum of electronic and ZPE= -945.905227
Sum of electronic and thermal Energies= -945.901706
Sum of electronic and thermal Enthalpies= -945.900762

Sum of electronic and thermal Free Energies= -945.931834

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	11.602	9.860	65.397

B,0,0.1273603939,2.305273693,2.3631643386
Cl,0,1.4742997218,3.0847551067,1.5613155734
Cl,0,-1.2482795945,1.7165262799,1.4558196424
H,0,0.1493954788,2.1727289204,3.5405624456

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.014370	E(Thermal)=	0.017939
E(QCISD(T))=	-944.685001	E(Empiric)=	-0.060840
DE(Plus)=	-0.004839	DE(2DF)=	-0.138077
E(Delta-G3)=	-0.736980	E(G3-Empiric)=	-0.060840
G3(0 K)=	-945.611367	G3 Energy=	-945.607798
G3 Enthalpy=	-945.606854	G3 Free Energy=	-945.638004

For Anharmonic Corrections of 5b-1

Zero-point vibrational energy 39311.3 (Joules/Mol)
9.39563 (Kcal/Mol)
Warning -- explicit consideration of 1 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 424.07 1053.67 1123.80 1291.22 1600.39
(Kelvin) 3962.97

Zero-point correction=	0.014973 (Hartree/Particle)
Thermal correction to Energy=	0.018495
Thermal correction to Enthalpy=	0.019439
Thermal correction to Gibbs Free Energy=	-0.011635
Sum of electronic and zero-point Energies=	-945.905222
Sum of electronic and thermal Energies=	-945.901700
Sum of electronic and thermal Enthalpies=	-945.900756
Sum of electronic and thermal Free Energies=	-945.931830

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	11.606	9.870	65.401

ZPE(harm) = 0.39311D+02 kJ/mol ZPE(anh)= 0.38984D+02 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.18348D-06	0.21062D-06	
QZvib	0.14146D+01	0.14232D+01	
Energy	0.48558D+02	0.48264D+02	kJ/mol
Enthalpy	0.51037D+02	0.50743D+02	kJ/mol
Entropy	0.27364D+03	0.27380D+03	J/(mol K)
Sp.Heat(V)	0.41296D+02	0.41575D+02	J/(mol K)
Sp.Heat(P)	0.49610D+02	0.49890D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.18348D-06	0.21062D-06	
QZvib	0.14146D+01	0.14232D+01	
Energy	0.48558D+02	0.48264D+02	kJ/mol
Enthalpy	0.51037D+02	0.50743D+02	kJ/mol
Entropy	0.27364D+03	0.27380D+03	J/(mol K)
Sp.Heat(V)	0.41296D+02	0.41575D+02	J/(mol K)
Sp.Heat(P)	0.49610D+02	0.49890D+02	J/(mol K)

5b-2 Complex

B3LYP/6-31+G**

E(RB+HF-LYP) = -1063.84776886

Zero-point correction= 0.095015 (Hartree/Particle)
Thermal correction to Energy= 0.104947
Thermal correction to Enthalpy= 0.105891
Thermal correction to Gibbs Free Energy= 0.052986
Sum of electronic and ZPE= -1063.752753
Sum of electronic and thermal Energies= -1063.742822
Sum of electronic and thermal Enthalpies= -1063.741877
Sum of electronic and thermal Free Energies= -1063.794783

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.242	28.630	103.784

C,0,0.5321063455,-0.4582397204,0.9721712091
C,0,1.7447312496,0.1000330148,0.9115976578
H,0,2.1333316022,0.5205695707,-0.0139914676
B,0,0.2922359647,2.7717876152,2.1998319911
Cl,0,0.2635260283,2.2443185319,3.8740682649
C,0,-0.4268409866,-0.5749393337,-0.1762423723

H,0,0.1924756559,-0.8727438268,1.9224016374
H,0,2.3994890427,0.1418554743,1.777788684
Cl,0,-1.2002561987,2.9704058129,1.2970747829
H,0,1.3200154642,3.0801621492,1.7014316998
H,0,-1.367622828,-0.0524360568,0.0424876352
H,0,-0.0080730453,-0.1528454298,-1.095639494
H,0,-0.6857372946,-1.6250078014,-0.3666602284

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.82992721

Zero-point correction= 0.095926 (Hartree/Particle)
Thermal correction to Energy= 0.105553
Thermal correction to Enthalpy= 0.106497
Thermal correction to Gibbs Free Energy= 0.056534
Sum of electronic and ZPE= -1063.734001
Sum of electronic and thermal Energies= -1063.724374
Sum of electronic and thermal Enthalpies= -1063.723430
Sum of electronic and thermal Free Energies= -1063.773393

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.235	28.640	105.157

C,0,0.2027779475,-0.4792425764,0.9994558981
C,0,1.3867362816,-0.4472016773,1.6183440019
C,0,2.7133879603,-0.2600254101,0.9422915893
B,0,-0.0761550479,2.6806159425,1.9008640919
Cl,0,1.4620022044,3.4128402239,1.4768133244
H,0,0.1207116158,-0.3712090883,-0.0804251484
H,0,-0.7242804394,-0.6321903076,1.545273149
H,0,1.4153736286,-0.5683017627,2.7021273592
Cl,0,-0.5146494299,2.4264276169,3.5817017138
H,0,-0.8600585682,2.4369292026,1.0488177609
H,0,3.2218022122,0.6388574976,1.3157628612
H,0,3.3810286537,-1.1078512891,1.145714989
H,0,2.6028329814,-0.1631583722,-0.1426915904

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.092089	E(Thermal)=	0.101882
E(QCISD(T))=	-1062.197487	E(Empiric)=	-0.121680
DE(Plus)=	-0.013347	DE(2DF)=	-0.255767
E(Delta-G3)=	-0.904834	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.401026	G3 Energy=	-1063.391234

G3 Enthalpy= -1063.390289 G3 Free Energy= -1063.440700

For Anharmonic Corrections of 5b-2

Zero-point vibrational energy 251032.2 (Joules/Mol)
59.99813 (Kcal/Mol)
Warning -- explicit consideration of 10 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 25.56 31.65 42.95 49.46 67.26
(Kelvin) 131.11 293.38 423.57 607.17 851.59
1048.32 1109.40 1284.02 1339.72 1347.53
1374.78 1486.92 1554.59 1596.39 1731.39
1925.54 2062.89 2116.81 2171.26 2190.49
2480.26 3977.78 4375.48 4446.10 4495.27
4534.34 4547.21 4664.21

Zero-point correction= 0.095613 (Hartree/Particle)
Thermal correction to Energy= 0.105535
Thermal correction to Enthalpy= 0.106479
Thermal correction to Gibbs Free Energy= 0.054395
Sum of electronic and zero-point Energies= -1063.733774
Sum of electronic and thermal Energies= -1063.723853
Sum of electronic and thermal Enthalpies= -1063.722908
Sum of electronic and thermal Free Energies= -1063.774992

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.224	28.746	109.620

ZPE(harm) = 0.25103D+03 kJ/mol ZPE(anh)= 0.24735D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.25080D-38	0.69064D-39	
QZvib	0.23890D+06	0.14889D+05	
Energy	0.27708D+03	0.26906D+03	kJ/mol
Enthalpy	0.27956D+03	0.27154D+03	kJ/mol
Entropy	0.45865D+03	0.43765D+03	J/(mol K)
Sp.Heat(V)	0.12027D+03	0.10500D+03	J/(mol K)
Sp.Heat(P)	0.12859D+03	0.11332D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value
Qvib	0.25080D-38	0.69064D-39

QZvib	0.23890D+06	0.14889D+05	
Energy	0.27708D+03	0.26906D+03	kJ/mol
Enthalpy	0.27956D+03	0.27154D+03	kJ/mol
Entropy	0.45865D+03	0.43765D+03	J/(mol K)
Sp.Heat(V)	0.12027D+03	0.10500D+03	J/(mol K)
Sp.Heat(P)	0.12859D+03	0.11332D+03	J/(mol K)

Starting Material

bcl3
B3LYP/6-31+G**
E(RB+HF-LYP) = -1405.56670087

Zero-point correction= 0.007584 (Hartree/Particle)
Thermal correction to Energy= 0.011961
Thermal correction to Enthalpy= 0.012906
Thermal correction to Gibbs Free Energy= -0.021625
Sum of electronic and ZPE= -1405.559117
Sum of electronic and thermal Energies= -1405.554740
Sum of electronic and thermal Enthalpies= -1405.553795
Sum of electronic and thermal Free Energies= -1405.588326

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	7.506	13.011	72.676

B,0,0.1280991186,2.3043596518,2.3699625987
Cl,0,1.4685291096,3.0831078937,1.5520404651
Cl,0,-1.2429862464,1.7203809706,1.4474532816
Cl,0,0.1596380182,2.108245484,4.1127226547

B3LYP/6-31G*
E(RB+HF-LYP) = -1405.56264100

Zero-point correction= 0.007618 (Hartree/Particle)
Thermal correction to Energy= 0.011993
Thermal correction to Enthalpy= 0.012937
Thermal correction to Gibbs Free Energy= -0.021589
Sum of electronic and ZPE= -1405.555023
Sum of electronic and thermal Energies= -1405.550648
Sum of electronic and thermal Enthalpies= -1405.549704
Sum of electronic and thermal Free Energies= -1405.584230

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	7.526	12.992	72.666

B,0,0.1282273437,2.3042052404,2.3704994854
Cl,0,1.4681594436,3.0829693905,1.5520603732
Cl,0,-1.2426872961,1.7205768626,1.4475123648
Cl,0,0.1595805089,2.1083425065,4.1121067766

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.007314	E(Thermal)=	0.011762
E(QCISD(T))=	-1403.775614	E(Empiric)=	-0.081120
DE(Plus)=	-0.006804	DE(2DF)=	-0.188923
E(Delta-G3)=	-1.081259	E(G3-Empiric)=	-0.081120
G3(0 K)=	-1405.126407	G3 Energy=	-1405.121958
G3 Enthalpy=	-1405.121014	G3 Free Energy=	-1405.155678

5b-3 Complex
B3LYP/6-31+G**
E(RB+HF-LYP) = -1063.84776886

Zero-point correction= 0.095015 (Hartree/Particle)
Thermal correction to Energy= 0.104947
Thermal correction to Enthalpy= 0.105891
Thermal correction to Gibbs Free Energy= 0.052986
Sum of electronic and ZPE= -1063.752753
Sum of electronic and thermal Energies= -1063.742822
Sum of electronic and thermal Enthalpies= -1063.741877
Sum of electronic and thermal Free Energies= -1063.794783

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.242	28.630	103.784

C,0,0.5321063455,-0.4582397204,0.9721712091
C,0,1.7447312496,0.1000330148,0.9115976578
H,0,2.1333316022,0.5205695707,-0.0139914676
B,0,0.2922359647,2.7717876152,2.1998319911
Cl,0,0.2635260283,2.2443185319,3.8740682649
C,0,-0.4268409866,-0.5749393337,-0.1762423723
H,0,0.1924756559,-0.8727438268,1.9224016374
H,0,2.3994890427,0.1418554743,1.777788684

Cl,0,-1.2002561987,2.9704058129,1.2970747829
H,0,1.3200154642,3.0801621492,1.7014316998
H,0,-1.367622828,-0.0524360568,0.0424876352
H,0,-0.0080730453,-0.1528454298,-1.095639494
H,0,-0.6857372946,-1.6250078014,-0.3666602284

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.82992721

Zero-point correction= 0.095926 (Hartree/Particle)
Thermal correction to Energy= 0.105553
Thermal correction to Enthalpy= 0.106497
Thermal correction to Gibbs Free Energy= 0.056534
Sum of electronic and ZPE= -1063.734001
Sum of electronic and thermal Energies= -1063.724374
Sum of electronic and thermal Enthalpies= -1063.723430
Sum of electronic and thermal Free Energies= -1063.773393

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.235	28.640	105.157

C,0,0.2027779475,-0.4792425764,0.9994558981
C,0,1.3867362816,-0.4472016773,1.6183440019
C,0,2.7133879603,-0.2600254101,0.9422915893
B,0,-0.0761550479,2.6806159425,1.9008640919
Cl,0,1.4620022044,3.4128402239,1.4768133244
H,0,0.1207116158,-0.3712090883,-0.0804251484
H,0,-0.7242804394,-0.6321903076,1.545273149
H,0,1.4153736286,-0.5683017627,2.7021273592
Cl,0,-0.5146494299,2.4264276169,3.5817017138
H,0,-0.8600585682,2.4369292026,1.0488177609
H,0,3.2218022122,0.6388574976,1.3157628612
H,0,3.3810286537,-1.1078512891,1.145714989
H,0,2.6028329814,-0.1631583722,-0.1426915904

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.092089	E(Thermal)=	0.101882
E(QCISD(T))=	-1062.197487	E(Empiric)=	-0.121680
DE(Plus)=	-0.013347	DE(2DF)=	-0.255767
E(Delta-G3)=	-0.904834	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.401026	G3 Energy=	-1063.391234
G3 Enthalpy=	-1063.390289	G3 Free Energy=	-1063.440700

For Anharmonic Corrections of 5b-3

Zero-point vibrational energy 251032.2 (Joules/Mol)
59.99813 (Kcal/Mol)
Warning -- explicit consideration of 10 degrees of freedom as vibrations may cause significant error
Vibrational temperatures: 25.56 31.65 42.95 49.46 67.26
(Kelvin) 131.11 293.38 423.57 607.17 851.59
1048.32 1109.40 1284.02 1339.72 1347.53
1374.78 1486.92 1554.59 1596.39 1731.39
1925.54 2062.89 2116.81 2171.26 2190.49
2480.26 3977.78 4375.48 4446.10 4495.27
4534.34 4547.21 4664.21

Zero-point correction= 0.095613 (Hartree/Particle)
Thermal correction to Energy= 0.105535
Thermal correction to Enthalpy= 0.106479
Thermal correction to Gibbs Free Energy= 0.054395
Sum of electronic and zero-point Energies= -1063.733774
Sum of electronic and thermal Energies= -1063.723853
Sum of electronic and thermal Enthalpies= -1063.722908
Sum of electronic and thermal Free Energies= -1063.774992

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.224	28.746	109.620

ZPE(harm) = 0.25103D+03 kJ/mol ZPE(anh)= 0.24735D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.25080D-38	0.69064D-39	
QZvib	0.23890D+06	0.14889D+05	
Energy	0.27708D+03	0.26906D+03	kJ/mol
Enthalpy	0.27956D+03	0.27154D+03	kJ/mol
Entropy	0.45865D+03	0.43765D+03	J/(mol K)
Sp.Heat(V)	0.12027D+03	0.10500D+03	J/(mol K)
Sp.Heat(P)	0.12859D+03	0.11332D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value
Qvib	0.25080D-38	0.69064D-39

QZvib	0.23890D+06	0.14889D+05	
Energy	0.27708D+03	0.26906D+03	kJ/mol
Enthalpy	0.27956D+03	0.27154D+03	kJ/mol
Entropy	0.45865D+03	0.43765D+03	J/(mol K)
Sp.Heat(V)	0.12027D+03	0.10500D+03	J/(mol K)
Sp.Heat(P)	0.12859D+03	0.11332D+03	J/(mol K)

5b-3 Complex
B3LYP/6-31+G**
E(RB+HF-LYP) = -1063.84787092

Zero-point correction= 0.095051 (Hartree/Particle)
Thermal correction to Energy= 0.104940
Thermal correction to Enthalpy= 0.105884
Thermal correction to Gibbs Free Energy= 0.054098
Sum of electronic and ZPE= -1063.752820
Sum of electronic and thermal Energies= -1063.742931
Sum of electronic and thermal Enthalpies= -1063.741987
Sum of electronic and thermal Free Energies= -1063.793773

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.216	28.754	108.440

C,0,0.2518819085,-0.7231277879,1.2127551896
C,0,1.4937548852,-0.5207168772,1.6662800688
C,0,2.7015499736,-0.2693697673,0.8098356336
B,0,-0.2116809447,2.8740964961,1.7934579457
H,0,-0.8464963135,2.3132923451,2.6182735686
Cl,0,1.3822472745,3.4840563523,2.1962109305
H,0,0.0259439777,-0.7203380135,0.1484621881
H,0,-0.5781099518,-0.9082069372,1.8886661407
H,0,1.66660982,-0.5374435235,2.743198831
Cl,0,-0.8969419945,3.1381039925,0.2028127402
H,0,3.1584675213,0.6989956298,1.0501895606
H,0,3.4706910679,-1.0324777044,0.983608055
H,0,2.4486717758,-0.2740812048,-0.2549958524

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.82980174

Zero-point correction= 0.095929 (Hartree/Particle)

Thermal correction to Energy= 0.105552
Thermal correction to Enthalpy= 0.106496
Thermal correction to Gibbs Free Energy= 0.056780
Sum of electronic and ZPE= -1063.733873
Sum of electronic and thermal Energies= -1063.724250
Sum of electronic and thermal Enthalpies= -1063.723306
Sum of electronic and thermal Free Energies= -1063.773022

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.235	28.639	104.636

C,0,0.2212079019,-0.5865681317,1.1680134646
C,0,1.4524236879,-0.4449398089,1.6669077308
C,0,2.6983762693,-0.2383987631,0.8559101348
B,0,-0.1471472477,2.6963444674,1.7879213797
H,0,-0.6721345876,2.1669423071,2.7067913331
Cl,0,1.4649127206,3.3639259437,1.98051726
H,0,0.0328091465,-0.5619653528,0.0965271101
H,0,-0.6416332612,-0.7473639744,1.8088485591
H,0,1.5886590249,-0.4835778346,2.7487265513
Cl,0,-1.0301718268,2.9086092308,0.2873456122
H,0,3.188455066,0.7075400326,1.1220739199
H,0,3.4282779045,-1.0364828233,1.0466067012
H,0,2.4825542017,-0.2212822927,-0.2174347567

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.092092	E(Thermal)=	0.101881
E(QCISD(T))=	-1062.197307	E(Empiric)=	-0.121680
DE(Plus)=	-0.013325	DE(2DF)=	-0.255702
E(Delta-G3)=	-0.904891	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.400813	G3 Energy=	-1063.391024
G3 Enthalpy=	-1063.390080	G3 Free Energy=	-1063.440243

For Anharmonic Corrections of 5b-3

Zero-point vibrational energy 251073.2 (Joules/Mol)
60.00794 (Kcal/Mol)
Warning -- explicit consideration of 10 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 28.05 34.19 50.50 58.52 70.67
(Kelvin) 127.60 290.83 423.46 607.74 851.19
1047.43 1105.84 1282.19 1339.64 1345.83
1374.32 1489.08 1555.78 1594.30 1732.06

1925.06 2062.21 2116.91 2170.31 2189.25
2479.43 3977.42 4376.34 4448.03 4496.05
4532.65 4547.58 4663.79

Zero-point correction= 0.095629 (Hartree/Particle)
Thermal correction to Energy= 0.105522
Thermal correction to Enthalpy= 0.106466
Thermal correction to Gibbs Free Energy= 0.054948
Sum of electronic and zero-point Energies= -1063.733936
Sum of electronic and thermal Energies= -1063.724043
Sum of electronic and thermal Enthalpies= -1063.723099
Sum of electronic and thermal Free Energies= -1063.774617

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.216	28.754	108.429

ZPE(harm) = 0.25107D+03 kJ/mol ZPE(anh)= 0.24834D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.15240D-38	0.17070D-38	
QZvib	0.14759D+06	0.54797D+05	
Energy	0.27705D+03	0.27392D+03	kJ/mol
Enthalpy	0.27953D+03	0.27640D+03	kJ/mol
Entropy	0.45367D+03	0.44412D+03	J/(mol K)
Sp.Heat(V)	0.12031D+03	0.12091D+03	J/(mol K)
Sp.Heat(P)	0.12862D+03	0.12923D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.15240D-38	0.17070D-38	
QZvib	0.14759D+06	0.54797D+05	
Energy	0.27705D+03	0.27392D+03	kJ/mol
Enthalpy	0.27953D+03	0.27640D+03	kJ/mol
Entropy	0.45367D+03	0.44412D+03	J/(mol K)
Sp.Heat(V)	0.12031D+03	0.12091D+03	J/(mol K)
Sp.Heat(P)	0.12862D+03	0.12923D+03	J/(mol K)

5b-4 Complex
B3LYP/6-31+G**
E(RB+HF-LYP) = -1063.84754811

Zero-point correction= 0.095015 (Hartree/Particle)
Thermal correction to Energy= 0.104947
Thermal correction to Enthalpy= 0.105891
Thermal correction to Gibbs Free Energy= 0.052986
Sum of electronic and ZPE= -1063.752753
Sum of electronic and thermal Energies= -1063.742822
Sum of electronic and thermal Enthalpies= -1063.741877
Sum of electronic and thermal Free Energies= -1063.794783

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.242	28.630	103.809

C,0,0.5321862474,-0.4590264591,0.9724144262
C,0,1.7443481557,0.1003028898,0.9122005234
H,0,2.1323272534,0.5223494255,-0.0129592485
B,0,0.2926639688,2.7719304591,2.1988984969
Cl,0,0.2634541205,2.2453627522,3.8734076974
C,0,-0.4270175147,-0.5749765977,-0.1758533646
H,0,0.1931790437,-0.8750498347,1.9222041395
H,0,2.399346504,0.1414932267,1.7782399366
Cl,0,-1.1995906645,2.9706381814,1.2957598611
H,0,1.3206377738,3.0797382796,1.7005438184
H,0,-1.3681428569,-0.0535026502,0.0438523803
H,0,-0.0088707214,-0.1513404416,-1.0948225874
H,0,-0.6851403099,-1.624999231,-0.3675660794

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.82967438

Zero-point correction= 0.095917 (Hartree/Particle)
Thermal correction to Energy= 0.105560
Thermal correction to Enthalpy= 0.106505
Thermal correction to Gibbs Free Energy= 0.056742
Sum of electronic and ZPE= -1063.733758
Sum of electronic and thermal Energies= -1063.724114
Sum of electronic and thermal Enthalpies= -1063.723170
Sum of electronic and thermal Free Energies= -1063.772933

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.240	28.634	104.735

C,0,0.2185765366,-0.5877026284,1.0330376665
C,0,1.4061178406,-0.4653961385,1.6326235327
C,0,2.7066091364,-0.1960847671,0.9322720915
B,0,-0.1094810309,2.6525582926,1.8812657755
Cl,0,-0.6235454274,2.4043827895,3.5407425404
H,0,1.0443826258,2.7457826561,1.6349109365
H,0,0.1116446245,-0.4968207584,-0.0461040748
H,0,-0.6876224643,-0.7962584771,1.5953096943
H,0,1.4604994633,-0.5707565492,2.7170476901
Cl,0,-1.2880451422,2.8802397869,0.6021372878
H,0,3.16919433,0.7305909043,1.2978928204
H,0,3.428951879,-1.001548395,1.1206868221
H,0,2.5701806287,-0.1060247157,-0.1504467832

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.092080	E(Thermal)=	0.101889
E(QCISD(T))=	-1062.197099	E(Empiric)=	-0.121680
DE(Plus)=	-0.013350	DE(2DF)=	-0.255638
E(Delta-G3)=	-0.904759	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.400447	G3 Energy=	-1063.390638
G3 Enthalpy=	-1063.389694	G3 Free Energy=	-1063.439903

For Anharmonic Corrections of 5b-4

Zero-point vibrational energy 251032.2 (Joules/Mol)
59.99813 (Kcal/Mol)
Warning -- explicit consideration of 10 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 25.56 31.65 42.95 49.46 67.26
(Kelvin) 131.11 293.38 423.57 607.17 851.59
1048.32 1109.40 1284.02 1339.72 1347.53
1374.78 1486.92 1554.59 1596.39 1731.39
1925.54 2062.89 2116.81 2171.26 2190.49
2480.26 3977.78 4375.48 4446.10 4495.27
4534.34 4547.21 4664.21

Zero-point correction=	0.095613 (Hartree/Particle)
Thermal correction to Energy=	0.105535
Thermal correction to Enthalpy=	0.106479
Thermal correction to Gibbs Free Energy=	0.054395
Sum of electronic and zero-point Energies=	-1063.733774
Sum of electronic and thermal Energies=	-1063.723853
Sum of electronic and thermal Enthalpies=	-1063.722908
Sum of electronic and thermal Free Energies=	-1063.774992

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.224	28.746	109.620

ZPE(harm) = 0.25103D+03 kJ/mol ZPE(anh)= 0.24735D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.25080D-38	0.69051D-39	
QZvib	0.23890D+06	0.14887D+05	
Energy	0.27708D+03	0.26906D+03	kJ/mol
Enthalpy	0.27956D+03	0.27154D+03	kJ/mol
Entropy	0.45865D+03	0.43765D+03	J/(mol K)
Sp.Heat(V)	0.12027D+03	0.10500D+03	J/(mol K)
Sp.Heat(P)	0.12859D+03	0.11332D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.25080D-38	0.69051D-39	
QZvib	0.23890D+06	0.14887D+05	
Energy	0.27708D+03	0.26906D+03	kJ/mol
Enthalpy	0.27956D+03	0.27154D+03	kJ/mol
Entropy	0.45865D+03	0.43765D+03	J/(mol K)
Sp.Heat(V)	0.12027D+03	0.10500D+03	J/(mol K)
Sp.Heat(P)	0.12859D+03	0.11332D+03	J/(mol K)

5b-5 Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -1063.82958495

Zero-point correction= 0.097651 (Hartree/Particle)
Thermal correction to Energy= 0.104753
Thermal correction to Enthalpy= 0.105697
Thermal correction to Gibbs Free Energy= 0.065572
Sum of electronic and ZPE= -1063.731440
Sum of electronic and thermal Energies= -1063.724337
Sum of electronic and thermal Enthalpies= -1063.723393
Sum of electronic and thermal Free Energies= -1063.763518

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 65.734 24.762 84.451

C,0,0.0486809455,0.0117202864,1.0675215821
C,0,1.2377220569,0.1185025104,1.8130667871
H,0,2.17502503,0.2312267124,1.2775665366
B,0,0.4555810397,1.6620466965,1.9901688982
Cl,0,1.4856660474,2.969853934,1.1919993524
C,0,-0.0062634095,0.0842006902,-0.4298155583
H,0,-0.8303000111,-0.3902348388,1.5683711515
H,0,1.2928053159,-0.3603032393,2.7842203031
Cl,0,-0.0330617035,1.9046142428,3.7521572421
H,0,-0.6000160522,1.6387234902,1.3571277287
H,0,-0.974680788,0.4370862579,-0.7919445199
H,0,0.7875304221,0.7204863121,-0.8275165706
H,0,0.1506911067,-0.9350030547,-0.8066029331

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.81199343

Zero-point correction= 0.098240 (Hartree/Particle)
Thermal correction to Energy= 0.105299
Thermal correction to Enthalpy= 0.106244
Thermal correction to Gibbs Free Energy= 0.066216
Sum of electronic and ZPE= -1063.713753
Sum of electronic and thermal Energies= -1063.706694
Sum of electronic and thermal Enthalpies= -1063.705750
Sum of electronic and thermal Free Energies= -1063.745778

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.076	24.572	84.245

C,0,0.0434506969,0.0171609993,1.0707699322
C,0,1.2348556827,0.1198859881,1.8181259118
H,0,2.1728089826,0.2203484877,1.2803637315
B,0,0.4640989266,1.6596854345,1.9924284069
Cl,0,1.4805080077,2.9632425044,1.1721832942
C,0,-0.0054903716,0.0892738888,-0.4276831282
H,0,-0.8349447545,-0.3906366882,1.5684923119
H,0,1.2892388754,-0.3697396815,2.7845297718
Cl,0,-0.0308803416,1.9140040308,3.7491858091
H,0,-0.5974375589,1.6261602241,1.3583211114
H,0,-0.9774998928,0.4290993329,-0.794482201
H,0,0.7803847391,0.7406970208,-0.8184044053

H,0,0.1702870083,-0.9262615418,-0.8075105462

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.094311	E(Thermal)=	0.101562
E(QCISD(T))=	-1062.178363	E(Empiric)=	-0.121680
DE(Plus)=	-0.012316	DE(2DF)=	-0.260051
E(Delta-G3)=	-0.904203	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.382302	G3 Energy=	-1063.375051
G3 Enthalpy=	-1063.374107	G3 Free Energy=	-1063.414503

For Anharmonic Corrections of 5b-5

Zero-point vibrational energy 257979.3 (Joules/Mol)
61.65853 (Kcal/Mol)
Warning -- explicit consideration of 8 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 125.02 255.88 286.68 329.23 415.46
(Kelvin) 531.03 613.41 723.25 1029.60 1062.44
1279.10 1325.09 1372.67 1383.88 1417.75
1532.98 1561.93 1704.85 1774.87 1872.73
2045.33 2092.58 2156.05 2186.93 2238.74
3418.27 4401.43 4508.05 4557.18 4566.41
4588.25 4698.42

Zero-point correction=	0.098259 (Hartree/Particle)
Thermal correction to Energy=	0.105370
Thermal correction to Enthalpy=	0.106314
Thermal correction to Gibbs Free Energy=	0.066125
Sum of electronic and zero-point Energies=	-1063.713743
Sum of electronic and thermal Energies=	-1063.706633
Sum of electronic and thermal Enthalpies=	-1063.705688
Sum of electronic and thermal Free Energies=	-1063.745877

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.121	24.650	84.585

ZPE(harm) = 0.25555D+03 kJ/mol ZPE(anh)= 0.25213D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value
Qvib	0.48046D-43	0.19983D-42
QZvib	0.28338D+02	0.29663D+02

Energy	0.27422D+03	0.27095D+03	kJ/mol
Enthalpy	0.27670D+03	0.27343D+03	kJ/mol
Entropy	0.36222D+03	0.36309D+03	J/(mol K)
Sp.Heat(V)	0.10313D+03	0.10444D+03	J/(mol K)
Sp.Heat(P)	0.11145D+03	0.11276D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.48046D-43	0.19983D-42	
QZvib	0.28338D+02	0.29663D+02	
Energy	0.27422D+03	0.27095D+03	kJ/mol
Enthalpy	0.27670D+03	0.27343D+03	kJ/mol
Entropy	0.36222D+03	0.36309D+03	J/(mol K)
Sp.Heat(V)	0.10313D+03	0.10444D+03	J/(mol K)
Sp.Heat(P)	0.11145D+03	0.11276D+03	J/(mol K)

5b-6 Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -1063.82993085

Zero-point correction= 0.097887 (Hartree/Particle)
Thermal correction to Energy= 0.104948
Thermal correction to Enthalpy= 0.105892
Thermal correction to Gibbs Free Energy= 0.066013
Sum of electronic and ZPE= -1063.724029
Sum of electronic and thermal Energies= -1063.716968
Sum of electronic and thermal Enthalpies= -1063.716024
Sum of electronic and thermal Free Energies= -1063.755903

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	65.856	24.657	83.932

C,0,0.0218078969,0.0451601726,1.0848257989
C,0,1.2440475629,0.0545080183,1.7813307038
C,0,2.5842195211,-0.0085866952,1.0794576469
B,0,0.471477147,1.6455797312,1.9165102836
Cl,0,1.5052449866,2.9393321002,1.125094812
H,0,0.0030849247,0.1413477725,0.0015430076
H,0,-0.8863062454,-0.3348366069,1.5432304475
H,0,1.2219916054,-0.3559437946,2.7871231251
Cl,0,-0.0520823919,1.9107637815,3.6635350841
H,0,-0.5737118077,1.6303949973,1.2565984405

H,0,3.3336383033,0.587752646,1.6065534125
H,0,2.9307125793,-1.0484667661,1.0559890251
H,0,2.5273859177,0.3594846433,0.0522582123

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.80495714

Zero-point correction= 0.098485 (Hartree/Particle)
Thermal correction to Energy= 0.105515
Thermal correction to Enthalpy= 0.106459
Thermal correction to Gibbs Free Energy= 0.066632
Sum of electronic and ZPE= -1063.706472
Sum of electronic and thermal Energies= -1063.699442
Sum of electronic and thermal Enthalpies= -1063.698498
Sum of electronic and thermal Free Energies= -1063.738325

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	66.212	24.489	83.823

C,0,0.021003245,0.0478649246,1.0856662148
C,0,1.2435420479,0.0599720796,1.7855355614
C,0,2.5824416482,-0.0072692331,1.0809933794
B,0,0.4800699216,1.6452284145,1.9203741207
Cl,0,1.5038847423,2.9388878912,1.1173395874
H,0,0.0042310095,0.1416849823,0.0017338564
H,0,-0.8875276395,-0.3378674022,1.5399224743
H,0,1.2203758387,-0.3607264585,2.7873241593
Cl,0,-0.0528436118,1.9141432554,3.6624474034
H,0,-0.5694929624,1.6216809259,1.2573180005
H,0,3.3351362923,0.5848160798,1.6091593848
H,0,2.9264062133,-1.0485150405,1.050851691
H,0,2.524283255,0.366589581,0.0553841666

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.094546	E(Thermal)=	0.101767
E(QCISD(T))=	-1062.172296	E(Empiric)=	-0.121680
DE(Plus)=	-0.012381	DE(2DF)=	-0.260401
E(Delta-G3)=	-0.904050	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.376262	G3 Energy=	-1063.369041
G3 Enthalpy=	-1063.368097	G3 Free Energy=	-1063.408291

For Anharmonic Corrections of 5b-6

Zero-point vibrational energy 258661.5 (Joules/Mol)

61.82159 (Kcal/Mol)
Warning -- explicit consideration of 8 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 144.42 271.34 295.00 321.80 392.64
(Kelvin) 589.63 607.56 648.87 1056.24 1110.42
1275.14 1294.05 1303.52 1380.60 1466.67
1591.03 1646.59 1739.49 1764.70 1898.58
2063.52 2097.61 2173.31 2190.40 2239.95
3376.75 4405.75 4503.25 4538.45 4552.92
4591.85 4687.54

Zero-point correction= 0.098519 (Hartree/Particle)
Thermal correction to Energy= 0.105588
Thermal correction to Enthalpy= 0.106532
Thermal correction to Gibbs Free Energy= 0.066592
Sum of electronic and zero-point Energies= -1063.706451
Sum of electronic and thermal Energies= -1063.699382
Sum of electronic and thermal Enthalpies= -1063.698437
Sum of electronic and thermal Free Energies= -1063.738378

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.258	24.545	84.061

ZPE(harm) = 0.25554D+03 kJ/mol ZPE(anh)= 0.25143D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.42006D-43	0.42113D-42	
QZvib	0.24632D+02	0.47119D+02	
Energy	0.27410D+03	0.27081D+03	kJ/mol
Enthalpy	0.27658D+03	0.27329D+03	kJ/mol
Entropy	0.36003D+03	0.36818D+03	J/(mol K)
Sp.Heat(V)	0.10269D+03	0.10513D+03	J/(mol K)
Sp.Heat(P)	0.11101D+03	0.11344D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.42006D-43	0.42113D-42	
QZvib	0.24632D+02	0.47119D+02	
Energy	0.27410D+03	0.27081D+03	kJ/mol
Enthalpy	0.27658D+03	0.27329D+03	kJ/mol
Entropy	0.36003D+03	0.36818D+03	J/(mol K)
Sp.Heat(V)	0.10269D+03	0.10513D+03	J/(mol K)

Sp.Heat(P) 0.11101D+03 0.11344D+03 J/(mol K)

5b-7 Variational Transition State

B3LYP/6-31G**
E(RB+HF-LYP) = -1063.84745473

Zero-point correction= 0.094660 (Hartree/Particle)
Thermal correction to Energy= 0.102061
Thermal correction to Enthalpy= 0.103005
Thermal correction to Gibbs Free Energy= 0.057838
Sum of electronic and zero-point Energies= -1063.752795
Sum of electronic and thermal Energies= -1063.745394
Sum of electronic and thermal Enthalpies= -1063.744449
Sum of electronic and thermal Free Energies= -1063.789616

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	64.044	22.846	95.062

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.82813941

Zero-point correction= 0.095232 (Hartree/Particle)
Thermal correction to Energy= 0.103598
Thermal correction to Enthalpy= 0.104542
Thermal correction to Gibbs Free Energy= 0.054718
Sum of electronic and ZPE= -1063.732908
Sum of electronic and thermal Energies= -1063.724542
Sum of electronic and thermal Enthalpies= -1063.723597
Sum of electronic and thermal Free Energies= -1063.773422

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	65.009	24.763	104.864

C,0,-2.86244,-0.81057,-1.04819
C,0,-3.20749,0.28619,-0.37241
C,0,-3.81315,0.30225,1.00213
B,0,1.56776,0.0828,0.59514
Cl,0,2.21082,-1.47341,0.11571
Cl,0,1.98931,1.54376,-0.2737
H,0,0.84178,0.1502,1.52891

H,0,-3.00238,-1.80608,-0.63102
H,0,-2.43132,-0.75818,-2.04452
H,0,-3.0497,1.26169,-0.8352
H,0,-3.1892,0.87079,1.705
H,0,-4.79816,0.78824,0.99523
H,0,-3.93654,-0.71102,1.39895

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.091422	E(Thermal)=	0.099931
E(QCISD(T))=	-1062.194003	E(Empiric)=	-0.121680
DE(Plus)=	-0.013083	DE(2DF)=	-0.254542
E(Delta-G3)=	-0.905491	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.397377	G3 Energy=	-1063.388868
G3 Enthalpy=	-1063.387924	G3 Free Energy=	-1063.438120

5b-8 Variational Transition State
B3LYP/6-31G*
E(RB+HF-LYP) = -1063.84757773

Zero-point correction= 0.095008 (Hartree/Particle)
Thermal correction to Energy= 0.103996
Thermal correction to Enthalpy= 0.104940
Thermal correction to Gibbs Free Energy= 0.055721
Sum of electronic and zero-point Energies= -1063.752569
Sum of electronic and thermal Energies= -1063.743582
Sum of electronic and thermal Enthalpies= -1063.742638
Sum of electronic and thermal Free Energies= -1063.791856

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.258	26.777	103.589

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.82901124

Zero-point correction= 0.095572 (Hartree/Particle)
Thermal correction to Energy= 0.104573
Thermal correction to Enthalpy= 0.105517
Thermal correction to Gibbs Free Energy= 0.055964
Sum of electronic and ZPE= -1063.733439

Sum of electronic and thermal Energies= -1063.724438
Sum of electronic and thermal Enthalpies= -1063.723494
Sum of electronic and thermal Free Energies= -1063.773047

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	65.621	26.715	104.293

C,0,2.01309,-0.84397,0.83285
C,0,2.47622,0.34562,0.44317
C,0,2.9781,0.67172,-0.93422
B,0,-1.61099,-0.06435,0.60858
Cl,0,-1.7819,-1.47093,-0.42112
Cl,0,-2.05629,1.53068,0.03483
H,0,-1.22294,-0.1961,1.71925
H,0,1.96296,-1.68967,0.14986
H,0,1.67679,-1.02207,1.85088
H,0,2.51039,1.16033,1.16824
H,0,2.40799,1.49789,-1.37973
H,0,4.02723,0.99564,-0.90447
H,0,2.90709,-0.19203,-1.60355

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.091749	E(Thermal)=	0.100905
E(QCISD(T))=	-1062.195639	E(Empiric)=	-0.121680
DE(Plus)=	-0.013286	DE(2DF)=	-0.255041
E(Delta-G3)=	-0.905040	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.398938	G3 Energy=	-1063.389782
G3 Enthalpy=	-1063.388838	G3 Free Energy=	-1063.438801

5b-9 Variational Transition State
B3LYP/6-31G**
E(RB+HF-LYP) = -1063.84756013

Zero-point correction= 0.094942 (Hartree/Particle)
Thermal correction to Energy= 0.103043
Thermal correction to Enthalpy= 0.103987
Thermal correction to Gibbs Free Energy= 0.058171
Sum of electronic and zero-point Energies= -1063.752618
Sum of electronic and thermal Energies= -1063.744517
Sum of electronic and thermal Enthalpies= -1063.743573
Sum of electronic and thermal Free Energies= -1063.789390

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	64.661	24.798	96.430

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.82894018

Zero-point correction= 0.095512 (Hartree/Particle)
Thermal correction to Energy= 0.103620
Thermal correction to Enthalpy= 0.104564
Thermal correction to Gibbs Free Energy= 0.058763
Sum of electronic and ZPE= -1063.733428
Sum of electronic and thermal Energies= -1063.725320
Sum of electronic and thermal Enthalpies= -1063.724376
Sum of electronic and thermal Free Energies= -1063.770177

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	65.022	24.738	96.396

C,0,2.05876,-0.86407,0.81271
C,0,2.54751,0.32117,0.44184
C,0,3.07059,0.6536,-0.92613
B,0,-1.59753,-0.06225,0.60325
Cl,0,-1.7819,-1.47093,-0.42112
Cl,0,-2.05629,1.53068,0.03483
H,0,-1.18829,-0.19108,1.70669
H,0,2.00137,-1.70111,0.11963
H,0,1.70745,-1.04738,1.82472
H,0,2.58784,1.12707,1.17636
H,0,2.51975,1.49427,-1.36881
H,0,4.12471,0.95902,-0.88123
H,0,2.99236,-0.20146,-1.60578

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.091691	E(Thermal)=	0.099952
E(QCISD(T))=	-1062.195514	E(Empiric)=	-0.121680
DE(Plus)=	-0.013277	DE(2DF)=	-0.254999
E(Delta-G3)=	-0.905063	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.398842	G3 Energy=	-1063.390581
G3 Enthalpy=	-1063.389637	G3 Free Energy=	-1063.435809

5b-10 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -1063.89127526

Zero-point correction= 0.100321 (Hartree/Particle)
Thermal correction to Energy= 0.108157
Thermal correction to Enthalpy= 0.109101
Thermal correction to Gibbs Free Energy= 0.066487
Sum of electronic and ZPE= -1063.790954
Sum of electronic and thermal Energies= -1063.783119
Sum of electronic and thermal Enthalpies= -1063.782174
Sum of electronic and thermal Free Energies= -1063.824788

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	67.869	26.166	89.688

C,0,1.2112130331,0.0374122546,2.0536896026
C,0,0.0643890434,0.1900929688,1.0158253516
B,0,-0.6785172458,1.5468808161,1.2951645597
Cl,0,-2.0913677598,1.6049917729,2.3610346261
C,0,0.6036307036,0.0393450746,-0.4199436617
Cl,0,-0.1059097861,3.0829904902,0.6284895885
H,0,1.9685843255,0.8184607096,1.9239957411
H,0,1.7054518409,-0.931771577,1.9205892967
H,0,-0.6532234311,-0.6191930944,1.2059517546
H,0,0.8435876112,0.0860985187,3.0839740132
H,0,1.087035436,-0.9368335655,-0.5425904992
H,0,1.3446045178,0.811477085,-0.65113355
H,0,-0.1958512886,0.1109585465,-1.1651128232

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.87516363

Zero-point correction= 0.101023 (Hartree/Particle)
Thermal correction to Energy= 0.108840
Thermal correction to Enthalpy= 0.109784
Thermal correction to Gibbs Free Energy= 0.067203
Sum of electronic and ZPE= -1063.774141
Sum of electronic and thermal Energies= -1063.766324
Sum of electronic and thermal Enthalpies= -1063.765380
Sum of electronic and thermal Free Energies= -1063.807961

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.298	26.034	89.619

C,0,1.2062764949,0.0356778197,2.0535634192
C,0,0.0625863232,0.1892298682,1.0135068704
B,0,-0.6772999133,1.5477585503,1.2945471759
Cl,0,-2.0733698054,1.6105501452,2.3814665882
C,0,0.6062154963,0.0400732027,-0.4197774722
Cl,0,-0.1135788808,3.0797021143,0.6114269768
H,0,1.9621931084,0.8198555568,1.9301650866
H,0,1.7044021827,-0.9318859253,1.9183995703
H,0,-0.655459774,-0.6205658441,1.2016311672
H,0,0.8346672531,0.0800266044,3.0832398822
H,0,1.095409595,-0.9339813132,-0.5412289889
H,0,1.3438456688,0.8164119634,-0.6498277536
H,0,-0.1922607487,0.1080572577,-1.1671785223

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.096982	E(Thermal)=	0.104988
E(QCISD(T))=	-1062.245643	E(Empiric)=	-0.121680
DE(Plus)=	-0.011700	DE(2DF)=	-0.258404
E(Delta-G3)=	-0.904369	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.444814	G3 Energy=	-1063.436809
G3 Enthalpy=	-1063.435864	G3 Free Energy=	-1063.478841

5b-11 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -1063.89428627

Zero-point correction= 0.100189 (Hartree/Particle)
Thermal correction to Energy= 0.107997
Thermal correction to Enthalpy= 0.108942
Thermal correction to Gibbs Free Energy= 0.066230
Sum of electronic and ZPE= -1063.794097
Sum of electronic and thermal Energies= -1063.786289
Sum of electronic and thermal Enthalpies= -1063.785345
Sum of electronic and thermal Free Energies= -1063.828057

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	67.769	25.774	89.895

H,0,1.1991921905,0.4341561863,1.8554581621
C,0,0.3433170154,0.2453981544,1.1866929738
B,0,0.926886735,0.0962839007,-0.2575093023
Cl,0,1.9353948371,1.3870627868,-0.9347453044
C,0,-0.528199634,-0.888739482,1.7507536908
Cl,0,0.6300206728,-1.3186824185,-1.2738335759
H,0,-0.2135722833,1.1966712595,1.2058104459
C,0,-1.0269202218,-0.6018299069,3.1716807685
H,0,-1.3860435156,-1.0550038581,1.0878856172
H,0,0.0419477278,-1.8256660668,1.7446877349
H,0,-1.6439077287,-1.4242459536,3.549118206
H,0,-0.1897393399,-0.4669016179,3.8669007592
H,0,-1.6331574553,0.311348016,3.2031418243

B3LYP/6-31G*
E(RB+HF-LYP) = -1063.87776110

Zero-point correction= 0.100876 (Hartree/Particle)
Thermal correction to Energy= 0.108669
Thermal correction to Enthalpy= 0.109613
Thermal correction to Gibbs Free Energy= 0.066880
Sum of electronic and ZPE= -1063.776885
Sum of electronic and thermal Energies= -1063.769092
Sum of electronic and thermal Enthalpies= -1063.768148
Sum of electronic and thermal Free Energies= -1063.810881

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.191	25.635	89.940

H,0,1.1992740531,0.4351924693,1.8580972443
C,0,0.3435301561,0.2471256773,1.1883840192
B,0,0.9257549434,0.0959174868,-0.2573414186
Cl,0,1.9345856401,1.3850199263,-0.9358827024
C,0,-0.5273814109,-0.8882203405,1.7501792134
Cl,0,0.6254105874,-1.3199619089,-1.2708023589
H,0,-0.2143343631,1.1982317514,1.2087797593
C,0,-1.0260222999,-0.602314558,3.1703125006
H,0,-1.3847458423,-1.054429758,1.0859120195
H,0,0.0436347581,-1.825153852,1.7425547843

H,0,-1.6431956164,-1.4255369504,3.5472729441
H,0,-0.1887256313,-0.4672685529,3.8661742258
H,0,-1.6325659744,0.3112496098,3.2024017695

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.096841	E(Thermal)=	0.104817
E(QCISD(T))=	-1062.246593	E(Empiric)=	-0.121680
DE(Plus)=	-0.011196	DE(2DF)=	-0.257941
E(Delta-G3)=	-0.905018	E(G3-Empiric)=	-0.121680
G3(0 K)=	-1063.445587	G3 Energy=	-1063.437610
G3 Enthalpy=	-1063.436666	G3 Free Energy=	-1063.479789

A. 5. Theoretical Structures from "Dynamics and Selectivity In The Hydroboration Of Chloro- and Ether- Subtituted Alkenes"

6a-1 Starting Material

B3LYP/6-31+G**
E(RB+HF-LYP) = -577.515826325

Zero-point correction= 0.071537 (Hartree/Particle)
Thermal correction to Energy= 0.076343
Thermal correction to Enthalpy= 0.077288
Thermal correction to Gibbs Free Energy= 0.043491
Sum of electronic and ZPE= -577.444289
Sum of electronic and thermal Energies= -577.439483
Sum of electronic and thermal Enthalpies= -577.438539
Sum of electronic and thermal Free Energies= -577.472335

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	47.906	15.523	71.130

C,0,0.0614444474,-0.0171462638,0.0325484511
H,0,-0.7328205998,0.6620761439,-0.2833734852
C,0,0.0645364169,-0.2281298344,1.5098697716
C,0,1.1300396072,-0.0039329222,2.2842565593
Cl,0,-0.2710699832,-1.5816214829,-0.8670847855
H,0,-0.8705703316,-0.5716514101,1.9483861255
H,0,2.0785238615,0.3281078795,1.8684869042
H,0,1.0874775043,-0.1426406948,3.3601986209
H,0,1.0224290772,0.3491985848,-0.330608162

B3LYP/6-31G*
E(RB+HF-LYP) = -577.501370780

Zero-point correction= 0.071930 (Hartree/Particle)
Thermal correction to Energy= 0.076722
Thermal correction to Enthalpy= 0.077666
Thermal correction to Gibbs Free Energy= 0.043900
Sum of electronic and ZPE= -577.429440
Sum of electronic and thermal Energies= -577.424649
Sum of electronic and thermal Enthalpies= -577.423704
Sum of electronic and thermal Free Energies= -577.457471

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	48.144	15.442	71.068

C,0,0.0613635042,-0.0178244788,0.033639159
H,0,-0.7310612737,0.663677852,-0.2845833485
C,0,0.064672788,-0.2289299562,1.510874142
C,0,1.1285039398,-0.0044808231,2.2829777161
Cl,0,-0.271663648,-1.5817996933,-0.865690514
H,0,-0.8714195604,-0.572593028,1.9476014156
H,0,2.0770929532,0.3293559286,1.8678986503
H,0,1.0898353315,-0.1422588688,3.3597410823
H,0,1.0226659653,0.3491130676,-0.3297783027

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.069053	E(Thermal)=	0.073952
E(QCISD(T))=	-576.546680	E(Empiric)=	-0.081120
DE(Plus)=	-0.009811	DE(2DF)=	-0.167881
E(Delta-G3)=	-0.511387	E(G3-Empiric)=	-0.081120
G3(0 K)=	-577.247826	G3 Energy=	-577.242928
G3 Enthalpy=	-577.241984	G3 Free Energy=	-577.275939

For Anharmonic Corrections of 6a-1

Zero-point vibrational energy 188854.1 (Joules/Mol)
45.13721 (Kcal/Mol)
Warning -- explicit consideration of 4 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 159.88 408.80 582.41 855.72 1061.95
(Kelvin) 1317.46 1375.79 1380.63 1484.22 1623.87
1782.84 1874.21 1926.09 2115.09 2178.91
2487.76 4462.45 4546.06 4552.85 4579.51
4671.28

Zero-point correction=	0.071931 (Hartree/Particle)
Thermal correction to Energy=	0.076722
Thermal correction to Enthalpy=	0.077667
Thermal correction to Gibbs Free Energy=	0.043900
Sum of electronic and zero-point Energies=	-577.429440
Sum of electronic and thermal Energies=	-577.424648
Sum of electronic and thermal Enthalpies=	-577.423704
Sum of electronic and thermal Free Energies=	-577.457471

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	48.144	15.442	71.068

ZPE(harm) = 0.18885D+03 kJ/mol ZPE(anh)= 0.18638D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.35450D-32	0.99085D-32	
QZvib	0.43190D+01	0.44450D+01	
Energy	0.20143D+03	0.19903D+03	kJ/mol
Enthalpy	0.20391D+03	0.20151D+03	kJ/mol
Entropy	0.29735D+03	0.29782D+03	J/(mol K)
Sp.Heat(V)	0.64608D+02	0.65356D+02	J/(mol K)
Sp.Heat(P)	0.72923D+02	0.73671D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.35450D-32	0.99085D-32	
QZvib	0.43190D+01	0.44450D+01	
Energy	0.20143D+03	0.19903D+03	kJ/mol
Enthalpy	0.20391D+03	0.20151D+03	kJ/mol
Entropy	0.29735D+03	0.29782D+03	J/(mol K)
Sp.Heat(V)	0.64608D+02	0.65356D+02	J/(mol K)
Sp.Heat(P)	0.72923D+02	0.73671D+02	J/(mol K)

6a-2 Starting Material

B3LYP/6-31+G**

E(RB+HF-LYP) = -577.515826697

Zero-point correction= 0.071538 (Hartree/Particle)
Thermal correction to Energy= 0.076343
Thermal correction to Enthalpy= 0.077288
Thermal correction to Gibbs Free Energy= 0.043494
Sum of electronic and ZPE= -577.444289
Sum of electronic and thermal Energies= -577.439483
Sum of electronic and thermal Enthalpies= -577.438539
Sum of electronic and thermal Free Energies= -577.472332

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	47.906	15.522	71.124

C,0,0.0069181821,-0.0852324387,0.0065838815

H,0,-0.3188042331,-1.0062041816,-0.4810448408
C,0,0.0595652693,-0.2252559998,1.4914302501
C,0,1.1558835997,0.0156921932,2.2161710829
Cl,0,-1.221379097,1.1784876056,-0.5043214731
H,0,-0.8577024681,-0.5547189552,1.9760014507
H,0,2.0806529142,0.3571411824,1.756866382
H,0,1.1649673902,-0.1235837567,3.2928452935
H,0,0.9648384426,0.2298703507,-0.4089880267

B3LYP/6-31G*
E(RB+HF-LYP) = -577.501370854

Zero-point correction= 0.071930 (Hartree/Particle)
Thermal correction to Energy= 0.076722
Thermal correction to Enthalpy= 0.077666
Thermal correction to Gibbs Free Energy= 0.043898
Sum of electronic and ZPE= -577.429441
Sum of electronic and thermal Energies= -577.424649
Sum of electronic and thermal Enthalpies= -577.423705
Sum of electronic and thermal Free Energies= -577.457473

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	48.144	15.442	71.070

C,0,0.0065734208,-0.0856218395,0.0077971705
H,0,-0.3194786322,-1.0059363771,-0.4825322109
C,0,0.0595036943,-0.2258073371,1.4925041651
C,0,1.1537208712,0.0164837049,2.2150859301
Cl,0,-1.2187073125,1.1808769756,-0.5026255912
H,0,-0.8581794823,-0.557481023,1.9751661298
H,0,2.0788925415,0.3586915587,1.7562439794
H,0,1.166909398,-0.1217231456,3.2924169881
H,0,0.9657055012,0.226713483,-0.4085125608

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.069052	E(Thermal)=	0.073951
E(QCISD(T))=	-576.546678	E(Empiric)=	-0.081120
DE(Plus)=	-0.009811	DE(2DF)=	-0.167880
E(Delta-G3)=	-0.511387	E(G3-Empiric)=	-0.081120
G3(0 K)=	-577.247824	G3 Energy=	-577.242925
G3 Enthalpy=	-577.241981	G3 Free Energy=	-577.275937

For Anharmonic Corrections of 6a-1

Zero-point vibrational energy 188851.7 (Joules/Mol)
45.13664 (Kcal/Mol)
Warning -- explicit consideration of 4 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 159.73 408.68 582.25 855.72 1061.82
(Kelvin) 1317.50 1375.82 1380.79 1484.31 1623.95
1782.80 1874.23 1926.14 2115.23 2178.82
2488.01 4462.18 4545.95 4552.77 4579.42
4671.09

Zero-point correction= 0.071930 (Hartree/Particle)
Thermal correction to Energy= 0.076722
Thermal correction to Enthalpy= 0.077666
Thermal correction to Gibbs Free Energy= 0.043898
Sum of electronic and zero-point Energies= -577.429441
Sum of electronic and thermal Energies= -577.424649
Sum of electronic and thermal Enthalpies= -577.423705
Sum of electronic and thermal Free Energies= -577.457472

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	48.144	15.442	71.070

ZPE(harm) = 0.18885D+03 kJ/mol ZPE(anh)= 0.18638D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.35517D-32	0.99080D-32	
QZvib	0.43230D+01	0.44437D+01	
Energy	0.20143D+03	0.19903D+03	kJ/mol
Enthalpy	0.20391D+03	0.20151D+03	kJ/mol
Entropy	0.29736D+03	0.29781D+03	J/(mol K)
Sp.Heat(V)	0.64609D+02	0.65356D+02	J/(mol K)
Sp.Heat(P)	0.72924D+02	0.73670D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.35517D-32	0.99080D-32	
QZvib	0.43230D+01	0.44437D+01	
Energy	0.20143D+03	0.19903D+03	kJ/mol
Enthalpy	0.20391D+03	0.20151D+03	kJ/mol
Entropy	0.29736D+03	0.29781D+03	J/(mol K)

Sp.Heat(V)	0.64609D+02	0.65356D+02	J/(mol K)
Sp.Heat(P)	0.72924D+02	0.73670D+02	J/(mol K)

6a-3 Starting Material

B3LYP/6-31+G**
E(RB+HF-LYP) = -577.513933948

Zero-point correction= 0.071351 (Hartree/Particle)
Thermal correction to Energy= 0.076099
Thermal correction to Enthalpy= 0.077043
Thermal correction to Gibbs Free Energy= 0.043442
Sum of electronic and ZPE= -577.442582
Sum of electronic and thermal Energies= -577.437835
Sum of electronic and thermal Enthalpies= -577.436891
Sum of electronic and thermal Free Energies= -577.470492

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	47.753	15.488	70.718

C,0,-0.0811073137,-0.000022023,1.2670419232
C,0,0.018549895,-0.0000785158,2.5964544029
C,0,1.2684387262,-0.0001438687,3.4273655693
H,0,1.3055121613,-0.8847680375,4.0693082435
H,0,-0.8869841405,-0.0000806491,3.2054852963
H,0,-1.0532456485,0.0000182294,0.7844522223
H,0,0.7955154955,-0.0000211254,0.6273356599
Cl,0,2.8151857431,-0.0001301343,2.4816961673
H,0,1.3055450816,0.8844161245,4.0693905153

B3LYP/6-31G*
E(RB+HF-LYP) = -577.499415064

Zero-point correction= 0.071740 (Hartree/Particle)
Thermal correction to Energy= 0.076476
Thermal correction to Enthalpy= 0.077421
Thermal correction to Gibbs Free Energy= 0.043833
Sum of electronic and ZPE= -577.427676
Sum of electronic and thermal Energies= -577.422939
Sum of electronic and thermal Enthalpies= -577.421995
Sum of electronic and thermal Free Energies= -577.455582

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	47.990	15.409	70.691

C,0,-0.0806871059,-0.0000218626,1.2691036142
C,0,0.0170778896,-0.0000785169,2.5958578695
C,0,1.2676635693,-0.0001438647,3.4261865269
H,0,1.3065090211,-0.8840008045,4.0704920884
H,0,-0.8876609191,-0.0000811248,3.2065054139
H,0,-1.0510948769,0.0000182018,0.7817389319
H,0,0.7963093719,-0.0000205225,0.6294937557
Cl,0,2.8127507079,-0.0001303796,2.4785782117
H,0,1.3065423421,0.883648874,4.0705735879

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.068870	E(Thermal)=	0.073715
E(QCISD(T))=	-576.545370	E(Empiric)=	-0.081120
DE(Plus)=	-0.009251	DE(2DF)=	-0.168048
E(Delta-G3)=	-0.512380	E(G3-Empiric)=	-0.081120
G3(0 K)=	-577.247299	G3 Energy=	-577.242454
G3 Enthalpy=	-577.241510	G3 Free Energy=	-577.275286

For Anharmonic Corrections of 6a-3

Zero-point vibrational energy 188351.2 (Joules/Mol)
45.01701 (Kcal/Mol)
Warning -- explicit consideration of 4 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 208.22 343.64 737.19 799.25 1039.09
(Kelvin) 1347.14 1362.31 1384.39 1465.40 1552.53
1743.65 1911.24 1930.89 2106.06 2157.00
2506.81 4428.83 4491.65 4522.52 4576.00
4692.99

Zero-point correction=	0.071739 (Hartree/Particle)
Thermal correction to Energy=	0.076476
Thermal correction to Enthalpy=	0.077420
Thermal correction to Gibbs Free Energy=	0.043832
Sum of electronic and zero-point Energies=	-577.427676
Sum of electronic and thermal Energies=	-577.422939
Sum of electronic and thermal Enthalpies=	-577.421995
Sum of electronic and thermal Free Energies=	-577.455583

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	47.989	15.409	70.691

ZPE(harm) = 0.18835D+03 kJ/mol ZPE(anh)= 0.18565D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.37244D-32	0.12063D-31	
QZvib	0.37044D+01	0.40276D+01	
Energy	0.20079D+03	0.19825D+03	kJ/mol
Enthalpy	0.20327D+03	0.20073D+03	kJ/mol
Entropy	0.29577D+03	0.29703D+03	J/(mol K)
Sp.Heat(V)	0.64471D+02	0.65515D+02	J/(mol K)
Sp.Heat(P)	0.72786D+02	0.73829D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.37244D-32	0.12063D-31	
QZvib	0.37044D+01	0.40276D+01	
Energy	0.20079D+03	0.19825D+03	kJ/mol
Enthalpy	0.20327D+03	0.20073D+03	kJ/mol
Entropy	0.29577D+03	0.29703D+03	J/(mol K)
Sp.Heat(V)	0.64471D+02	0.65515D+02	J/(mol K)
Sp.Heat(P)	0.72786D+02	0.73829D+02	J/(mol K)

6a-4 Complex

B3LYP/6-31G*

E(RB+HF-LYP) = -604.127511711

Zero-point correction= 0.104049 (Hartree/Particle)
Thermal correction to Energy= 0.110883
Thermal correction to Enthalpy= 0.111827
Thermal correction to Gibbs Free Energy= 0.073323
Sum of electronic and ZPE= -604.023463
Sum of electronic and thermal Energies= -604.016628
Sum of electronic and thermal Enthalpies= -604.015684
Sum of electronic and thermal Free Energies= -604.054189

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.580	23.733	81.040

C,0,0.0277506016,-0.0310932454,1.0300815972

B,0,0.3146929602,1.7138491982,1.8181209833
C,0,1.228163969,0.0058427521,1.6857721413
C,0,2.5952420509,0.0416566328,1.0493836797
H,0,-0.0148954249,0.0502262307,-0.049928962
H,0,-0.8762332111,-0.3466228756,1.5375294277
H,0,1.265856513,-0.2793482361,2.7345545111
H,0,-0.0492260639,1.706372086,2.9591633798
H,0,-0.5609433016,1.9930717208,1.0295691265
H,0,1.3043724619,2.3172870605,1.5077568764
H,0,3.2422637454,0.7628541626,1.5498501956
H,0,3.04846239,-0.9513550301,1.1314446592
Cl,0,2.6053533093,0.4599695437,-0.7075176159

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.099880	E(Thermal)=	0.106912
E(QCISD(T))=	-603.045726	E(Empiric)=	-0.101400
DE(Plus)=	-0.009638	DE(2DF)=	-0.210052
E(Delta-G3)=	-0.561252	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.828189	G3 Energy=	-603.821157
G3 Enthalpy=	-603.820213	G3 Free Energy=	-603.859112

For Anharmonic Corrections of 6a-4

Zero-point vibrational energy 273164.0 (Joules/Mol)
65.28776 (Kcal/Mol)
Warning -- explicit consideration of 7 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 136.39 140.31 305.27 387.68 473.01
(Kelvin) 639.52 741.45 1034.07 1046.91 1053.40
1232.79 1355.25 1377.38 1466.35 1492.06
1585.19 1589.04 1682.39 1702.31 1757.36
1897.57 1936.65 2098.84 2153.83 2354.83
3625.54 3711.39 3812.70 4445.74 4548.33
4587.48 4604.29 4732.78

Zero-point correction=	0.104043 (Hartree/Particle)
Thermal correction to Energy=	0.110890
Thermal correction to Enthalpy=	0.111834
Thermal correction to Gibbs Free Energy=	0.073282
Sum of electronic and zero-point Energies=	-604.023500
Sum of electronic and thermal Energies=	-604.016653
Sum of electronic and thermal Enthalpies=	-604.015709
Sum of electronic and thermal Free Energies=	-604.054260

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.584	23.759	81.139

ZPE(harm) = 0.27316D+03 kJ/mol ZPE(anh)= 0.26989D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.39786D-46	0.10577D-45	
QZvib	0.28572D+02	0.20304D+02	
Energy	0.29114D+03	0.28783D+03	kJ/mol
Enthalpy	0.29362D+03	0.29031D+03	kJ/mol
Entropy	0.33948D+03	0.33650D+03	J/(mol K)
Sp.Heat(V)	0.99407D+02	0.10122D+03	J/(mol K)
Sp.Heat(P)	0.10772D+03	0.10953D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.39786D-46	0.10577D-45	
QZvib	0.28572D+02	0.20304D+02	
Energy	0.29114D+03	0.28783D+03	kJ/mol
Enthalpy	0.29362D+03	0.29031D+03	kJ/mol
Entropy	0.33948D+03	0.33650D+03	J/(mol K)
Sp.Heat(V)	0.99407D+02	0.10122D+03	J/(mol K)
Sp.Heat(P)	0.10772D+03	0.10953D+03	J/(mol K)

6a-5 Complex

B3LYP/6-31+G**

E(RB+HF-LYP) = -604.146593505

Zero-point correction= 0.103403 (Hartree/Particle)
Thermal correction to Energy= 0.110331
Thermal correction to Enthalpy= 0.111276
Thermal correction to Gibbs Free Energy= 0.072491
Sum of electronic and ZPE= -604.043190
Sum of electronic and thermal Energies= -604.036262
Sum of electronic and thermal Enthalpies= -604.035318
Sum of electronic and thermal Free Energies= -604.074102

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	69.234	23.931	81.629

C,0,0.0265142394,0.0772488394,0.0372495752
H,0,-0.8710831551,0.5412777373,-0.3686433023
C,0,0.0066646354,0.0167471423,1.5386898449
B,0,0.3982402244,1.7471117261,2.2704493202
C,0,1.1541637094,0.0484138173,2.3031868086
Cl,0,0.0760295062,-1.6171723825,-0.63747104
H,0,-0.9254539259,-0.3086024282,1.9910561167
H,0,2.1266460443,0.1234824198,1.8296627373
H,0,1.1412274927,-0.2961745722,3.3293149248
H,0,0.1786668563,1.9029751,3.4372661485
H,0,-0.6578105033,1.8947574855,1.6835732546
H,0,1.2479171254,2.361275192,1.6907970129
H,0,0.9114477508,0.5951899232,-0.3320214014

B3LYP/6-31G*
E(RB+HF-LYP) = -604.131119409

Zero-point correction= 0.104137 (Hartree/Particle)
Thermal correction to Energy= 0.111006
Thermal correction to Enthalpy= 0.111950
Thermal correction to Gibbs Free Energy= 0.073465
Sum of electronic and ZPE= -604.026982
Sum of electronic and thermal Energies= -604.020114
Sum of electronic and thermal Enthalpies= -604.019169
Sum of electronic and thermal Free Energies= -604.057655

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.657	23.772	80.999

C,0,0.1534297067,0.0030258961,1.5171470846
B,0,0.5383749638,1.8333234969,1.847961174
C,0,1.4616918434,0.2140937385,1.8999670369
C,0,2.6013241022,0.2362803433,0.9218947601
Cl,0,3.4044899465,-1.4072786944,0.8604744231
H,0,2.2662750724,0.4620726375,-0.0905621176
H,0,-0.1089504434,-0.1154795215,0.4702553233
H,0,-0.6005561067,-0.2951385347,2.2370510435
H,0,1.7358385538,0.0641859334,2.9391063244
H,0,-0.616554573,1.8258731661,1.4596774257
H,0,1.1909379656,2.4047948577,1.0186139559
H,0,0.5720173462,2.1538569062,3.0004642079
H,0,3.3797546224,0.9402437749,1.2137283583

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.099972	E(Thermal)=	0.107025
E(QCISD(T))=	-603.048352	E(Empiric)=	-0.101400
DE(Plus)=	-0.010097	DE(2DF)=	-0.209818
E(Delta-G3)=	-0.560186	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.829883	G3 Energy=	-603.822829
G3 Enthalpy=	-603.821885	G3 Free Energy=	-603.860723

For Anharmonic Corrections of 6a-5

Zero-point vibrational energy 273413.5 (Joules/Mol)
65.34739 (Kcal/Mol)
Warning -- explicit consideration of 7 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 137.37 195.48 270.58 351.97 459.88
(Kelvin) 594.97 752.00 987.34 1019.07 1122.07
1292.20 1353.06 1380.73 1488.84 1530.33
1589.87 1618.27 1660.07 1709.83 1797.97
1864.14 1910.68 2107.94 2180.43 2311.95
3548.60 3692.34 3826.89 4501.74 4580.77
4591.76 4628.45 4710.50

Zero-point correction= 0.104138 (Hartree/Particle)
Thermal correction to Energy= 0.111006
Thermal correction to Enthalpy= 0.111950
Thermal correction to Gibbs Free Energy= 0.073466
Sum of electronic and zero-point Energies= -604.026982
Sum of electronic and thermal Energies= -604.020113
Sum of electronic and thermal Enthalpies= -604.019169
Sum of electronic and thermal Free Energies= -604.057654

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.657	23.772	80.998

ZPE(harm) = 0.27341D+03 kJ/mol ZPE(anh)= 0.26908D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.32386D-46	0.39807D-44	
QZvib	0.25720D+02	0.54987D+03	
Energy	0.29145D+03	0.28915D+03	kJ/mol
Enthalpy	0.29393D+03	0.29163D+03	kJ/mol

Entropy	0.33890D+03	0.37120D+03	J/(mol K)
Sp.Heat(V)	0.99463D+02	0.10267D+03	J/(mol K)
Sp.Heat(P)	0.10778D+03	0.11098D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.32386D-46	0.39807D-44	
QZvib	0.25720D+02	0.54987D+03	
Energy	0.29145D+03	0.28915D+03	kJ/mol
Enthalpy	0.29393D+03	0.29163D+03	kJ/mol
Entropy	0.33890D+03	0.37120D+03	J/(mol K)
Sp.Heat(V)	0.99463D+02	0.10267D+03	J/(mol K)
Sp.Heat(P)	0.10778D+03	0.11098D+03	J/(mol K)

6a-6 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.146426208

Zero-point correction= 0.103125 (Hartree/Particle)
Thermal correction to Energy= 0.109266
Thermal correction to Enthalpy= 0.110211
Thermal correction to Gibbs Free Energy= 0.073177
Sum of electronic and ZPE= -604.043301
Sum of electronic and thermal Energies= -604.037160
Sum of electronic and thermal Enthalpies= -604.036216
Sum of electronic and thermal Free Energies= -604.073250

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.566	21.740	77.945

C,0,0.0098930448,0.0546369195,0.0302194571
H,0,-0.8992005633,0.4904805433,-0.3828327773
C,0,-0.0108195464,0.0069522331,1.534863543
B,0,0.4562706157,1.6364003578,2.3184861549
C,0,1.1578833676,0.0080601686,2.2990622164
Cl,0,0.1111535016,-1.6408690125,-0.6282522963
H,0,-0.9334724645,-0.351312268,1.9826328846
H,0,2.1204866644,0.0326919387,1.8001958671
H,0,1.14736722,-0.4123381816,3.2969800234
H,0,0.1273967794,1.8272006618,3.4529468502
H,0,-0.59499481,1.7185562355,1.6817360383

H,0,1.2398487913,2.3205419816,1.7257606805
H,0,0.8813573996,0.5955284224,-0.3386886419

B3LYP/6-31G*
E(RB+HF-LYP) = -604.128055199

Zero-point correction= 0.104503 (Hartree/Particle)
Thermal correction to Energy= 0.110491
Thermal correction to Enthalpy= 0.111435
Thermal correction to Gibbs Free Energy= 0.074528
Sum of electronic and ZPE= -604.023552
Sum of electronic and thermal Energies= -604.017565
Sum of electronic and thermal Enthalpies= -604.016620
Sum of electronic and thermal Free Energies= -604.053527

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.334	21.258	77.677

C,0,0.069147191,0.2363712302,0.012224467
H,0,1.0199540578,0.6784154016,-0.2828582515
C,0,-0.0159475273,0.0253776214,1.4970943446
B,0,0.3387623453,1.6272395426,2.288852038
C,0,1.0830876825,0.0351877546,2.3344275328
Cl,0,-0.0596692421,-1.377191254,-0.8360587578
H,0,-0.751809534,0.8447529123,-0.366504395
H,0,-0.9480323848,-0.3991091937,1.8557386209
H,0,2.0822706849,0.1858751827,1.9378161824
H,0,1.0328168001,-0.4456789936,3.3046700743
H,0,0.7321068626,1.7161811449,3.4241917377
H,0,-0.8479716447,1.7936583281,2.4348869937
H,0,0.8879367088,2.337538323,1.4959474129

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.099805	E(Thermal)=	0.106108
E(QCISD(T))=	-603.047887	E(Empiric)=	-0.101400
DE(Plus)=	-0.009967	DE(2DF)=	-0.210027
E(Delta-G3)=	-0.560583	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.830059	G3 Energy=	-603.823756
G3 Enthalpy=	-603.822811	G3 Free Energy=	-603.860037

For Anharmonic Corrections of 6a-7

Zero-point vibrational energy 272652.6 (Joules/Mol)

65.16555 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 136.18 253.43 359.70 549.47 601.55
(Kelvin) 876.55 1011.76 1044.49 1165.36 1275.54
1316.62 1365.90 1472.19 1536.13 1605.75
1624.08 1673.57 1704.93 1791.01 1846.13
1913.83 2100.23 2182.50 2262.09 3408.19
3693.98 3844.80 4495.33 4575.98 4583.01
4612.63 4702.14

Zero-point correction= 0.103848 (Hartree/Particle)
Thermal correction to Energy= 0.109923
Thermal correction to Enthalpy= 0.110867
Thermal correction to Gibbs Free Energy= 0.073968
Sum of electronic and zero-point Energies= -604.026049
Sum of electronic and thermal Energies= -604.019974
Sum of electronic and thermal Enthalpies= -604.019030
Sum of electronic and thermal Free Energies= -604.055929

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.977	21.491	77.660

ZPE(harm) = 0.27066D+03 kJ/mol ZPE(anh)= 0.26613D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.44082D-46	0.29609D-45	
QZvib	0.11524D+02	0.12461D+02	
Energy	0.28661D+03	0.28235D+03	kJ/mol
Enthalpy	0.28909D+03	0.28482D+03	kJ/mol
Entropy	0.33324D+03	0.33478D+03	J/(mol K)
Sp.Heat(V)	0.89917D+02	0.91890D+02	J/(mol K)
Sp.Heat(P)	0.98231D+02	0.10020D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.44082D-46	0.29609D-45	
QZvib	0.11524D+02	0.12461D+02	
Energy	0.28661D+03	0.28235D+03	kJ/mol
Enthalpy	0.28909D+03	0.28482D+03	kJ/mol
Entropy	0.33324D+03	0.33478D+03	J/(mol K)
Sp.Heat(V)	0.89917D+02	0.91890D+02	J/(mol K)
Sp.Heat(P)	0.98231D+02	0.10020D+03	J/(mol K)

6a-7 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.142306143

Zero-point correction= 0.103201 (Hartree/Particle)
Thermal correction to Energy= 0.109207
Thermal correction to Enthalpy= 0.110151
Thermal correction to Gibbs Free Energy= 0.073479
Sum of electronic and ZPE= -604.039105
Sum of electronic and thermal Energies= -604.033099
Sum of electronic and thermal Enthalpies= -604.032155
Sum of electronic and thermal Free Energies= -604.068827

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.528	21.542	77.182

C,0,0.0697963532,-0.1165159235,0.0054958543
Cl,0,1.4752876473,0.6337697215,-0.8435504177
C,0,0.1129763957,-0.0358439375,1.5135844627
B,0,0.3419559355,1.6125754825,2.3636882187
C,0,1.2619347337,0.095961589,2.2950689438
H,0,0.0705410649,-1.1742853811,-0.2727195008
H,0,-0.8286744659,0.353512429,-0.3954197141
H,0,-0.7657439407,-0.4929101694,1.9654685904
H,0,2.2180456028,0.2552223827,1.8113589108
H,0,1.2831662727,-0.3335106901,3.2886083646
H,0,-0.0958402053,1.6859619475,3.4750151088
H,0,-0.6403793957,1.5923983575,1.6230107215
H,0,1.0711690016,2.4253491919,1.8791424571

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.099784	E(Thermal)=	0.105880
E(QCISD(T))=	-603.043682	E(Empiric)=	-0.101400
DE(Plus)=	-0.009991	DE(2DF)=	-0.210650
E(Delta-G3)=	-0.560812	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.826750	G3 Energy=	-603.820655
G3 Enthalpy=	-603.819710	G3 Free Energy=	-603.856515

For Anharmonic Corrections of 6a-7

Zero-point vibrational energy 272715.5 (Joules/Mol)
65.18057 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as

```
        vibrations may cause significant error
Vibrational temperatures:   144.30   251.19   368.42   567.26   716.89
      (Kelvin)          824.95  1003.88  1056.67  1133.87  1263.87
                       1338.01  1363.51  1459.77  1522.70  1572.48
                       1632.90  1661.83  1710.07  1760.67  1865.32
                       1936.21  2082.27  2152.08  2260.22  3470.74
                       3714.17  3866.13  4455.75  4551.41  4568.18
                       4597.88  4726.60

Zero-point correction=                          0.103872 (Hartree/Particle)
Thermal correction to Energy=                   0.109881
Thermal correction to Enthalpy=                 0.110825
Thermal correction to Gibbs Free Energy=        0.074092
Sum of electronic and zero-point Energies=          -604.021896
Sum of electronic and thermal Energies=             -604.015887
Sum of electronic and thermal Enthalpies=           -604.014943
Sum of electronic and thermal Free Energies=        -604.051675

                 E (Thermal)          CV                S
                  KCal/Mol       Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total               68.951          21.421            77.310

ZPE(harm) = 0.27073D+03 kJ/mol       ZPE(anh)= 0.26610D+03 kJ/mol

Input values of T(K) and P(atm): 298.15   1.00
             Harmonic value     SPT anharmonic value
Qvib          0.38929D-46         0.34232D-45
QZvib         0.10456D+02         0.14240D+02
Energy        0.28650D+03         0.28240D+03        kJ/mol
Enthalpy      0.28898D+03         0.28487D+03        kJ/mol
Entropy       0.33178D+03         0.33608D+03        J/(mol K)
Sp.Heat(V)     0.89624D+02         0.92017D+02       J/(mol K)
Sp.Heat(P)     0.97939D+02         0.10033D+03       J/(mol K)

T =  298.15 K;  P =   1.00 atm
             Harmonic value     SPT anharmonic value
Qvib          0.38929D-46         0.34232D-45
QZvib         0.10456D+02         0.14240D+02
Energy        0.28650D+03         0.28240D+03        kJ/mol
Enthalpy      0.28898D+03         0.28487D+03        kJ/mol
Entropy       0.33178D+03         0.33608D+03        J/(mol K)
Sp.Heat(V)     0.89624D+02         0.92017D+02       J/(mol K)
Sp.Heat(P)     0.97939D+02         0.10033D+03       J/(mol K)
```

6a-8 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.127220068

Zero-point correction= 0.103236 (Hartree/Particle)
Thermal correction to Energy= 0.109309
Thermal correction to Enthalpy= 0.110253
Thermal correction to Gibbs Free Energy= 0.073591
Sum of electronic and ZPE= -604.038510
Sum of electronic and thermal Energies= -604.032437
Sum of electronic and thermal Enthalpies= -604.031493
Sum of electronic and thermal Free Energies= -604.068155

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.593	21.946	77.162

C,0,-0.2032862384,0.036734594,0.0829076079
H,0,0.6607643455,-0.28307025,-0.5012082045
C,0,0.0631425009,-0.1171444804,1.5676674325
C,0,1.2935060148,0.1427349999,2.1277765191
B,0,0.200993219,1.6481695899,2.392273727
H,0,-0.4548318632,1.0636492474,-0.1800714626
Cl,0,-1.593201665,-0.999319851,-0.4405460209
H,0,-0.6796030467,-0.6664637684,2.1360497229
H,0,2.1260437839,0.469244159,1.5144408356
H,0,1.5399819886,-0.2392620275,3.1101835114
H,0,0.3327556778,1.7381532621,3.5797430246
H,0,-0.9836991751,1.5245102219,2.1628223319
H,0,0.6964574579,2.437542303,1.6373869751

B3LYP/6-31G*
E(RB+HF-LYP) = -604.125504486

Zero-point correction= 0.103953 (Hartree/Particle)
Thermal correction to Energy= 0.109975
Thermal correction to Enthalpy= 0.110919
Thermal correction to Gibbs Free Energy= 0.074389
Sum of electronic and ZPE= -604.021551
Sum of electronic and thermal Energies= -604.015529
Sum of electronic and thermal Enthalpies= -604.014585
Sum of electronic and thermal Free Energies= -604.051116

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	69.010	21.780	76.885

C,0,-0.2016675057,0.0350135746,0.0832752992
H,0,0.6562805871,-0.2929302374,-0.5066095011
C,0,0.0702252179,-0.1266124466,1.5663764193
C,0,1.296345652,0.1410296121,2.1257630009
B,0,0.1881389121,1.6501389408,2.3900352675
H,0,-0.4380159716,1.0673307071,-0.174562621
Cl,0,-1.6078947917,-0.9781068687,-0.4370429893
H,0,-0.6688162814,-0.6807824686,2.135063253
H,0,2.1271956461,0.4799318773,1.5160010845
H,0,1.5466259732,-0.2378807514,3.1090595488
H,0,0.3513951567,1.7409368904,3.5746196922
H,0,-1.0005811551,1.5244948364,2.1825251054
H,0,0.6797915604,2.4329143339,1.6249224406

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.099795	E(Thermal)=	0.105998
E(QCISD(T))=	-603.043371	E(Empiric)=	-0.101400
DE(Plus)=	-0.009917	DE(2DF)=	-0.209664
E(Delta-G3)=	-0.560591	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.825147	G3 Energy=	-603.818945
G3 Enthalpy=	-603.818000	G3 Free Energy=	-603.854846

For Anharmonic Corrections of 6a-7

Zero-point vibrational energy 272891.8 (Joules/Mol)
65.22270 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 190.35 348.54 362.61 491.22 542.17
(Kelvin) 730.91 1019.73 1076.17 1128.50 1227.63
1336.64 1359.15 1445.08 1523.88 1598.83
1643.30 1694.71 1698.41 1736.96 1880.25
1901.59 2104.91 2161.40 2304.52 3592.99
3693.83 3820.68 4490.78 4578.44 4594.26
4639.79 4724.40

Zero-point correction=	0.103939 (Hartree/Particle)
Thermal correction to Energy=	0.109993
Thermal correction to Enthalpy=	0.110937

Thermal correction to Gibbs Free Energy= 0.074291
Sum of electronic and zero-point Energies= -604.021543
Sum of electronic and thermal Energies= -604.015489
Sum of electronic and thermal Enthalpies= -604.014545
Sum of electronic and thermal Free Energies= -604.051191

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.021	21.804	77.129

ZPE(harm) = 0.27224D+03 kJ/mol ZPE(anh)= 0.26827D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.16747D-46	0.23417D-45	
QZvib	0.82936D+01	0.23336D+02	
Energy	0.28814D+03	0.28522D+03	kJ/mol
Enthalpy	0.29062D+03	0.28770D+03	kJ/mol
Entropy	0.33102D+03	0.34317D+03	J/(mol K)
Sp.Heat(V)	0.91229D+02	0.93998D+02	J/(mol K)
Sp.Heat(P)	0.99544D+02	0.10231D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.16747D-46	0.23417D-45	
QZvib	0.82936D+01	0.23336D+02	
Energy	0.28814D+03	0.28522D+03	kJ/mol
Enthalpy	0.29062D+03	0.28770D+03	kJ/mol
Entropy	0.33102D+03	0.34317D+03	J/(mol K)
Sp.Heat(V)	0.91229D+02	0.93998D+02	J/(mol K)
Sp.Heat(P)	0.99544D+02	0.10231D+03	J/(mol K)

6a-9 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.142936130

Zero-point correction= 0.103301 (Hartree/Particle)
Thermal correction to Energy= 0.109320
Thermal correction to Enthalpy= 0.110264
Thermal correction to Gibbs Free Energy= 0.073606
Sum of electronic and ZPE= -604.039635

Sum of electronic and thermal Energies= -604.033617
Sum of electronic and thermal Enthalpies= -604.032672
Sum of electronic and thermal Free Energies= -604.069330

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.599	21.566	77.152

C,0,0.0830397818,-0.1520669105,1.4317515858
C,0,1.2952960966,0.2893328883,1.9610840814
C,0,2.6361083158,0.2085773322,1.2609602487
H,0,3.1962627036,-0.6504948173,1.6391961905
B,0,0.265468003,1.6881594232,1.5635902894
H,0,0.0231796603,-0.4856188176,0.4016865128
H,0,-0.7249838472,-0.4559018711,2.0868709503
H,0,1.4042337787,0.2863882734,3.0428676722
H,0,-0.0442735489,2.1726375467,2.6125212738
H,0,-0.7733994965,1.3823855584,0.9823202673
H,0,0.9071168163,2.2608902501,0.7330270049
Cl,0,2.5422275716,-0.0174020504,-0.534827514
H,0,3.2213481647,1.1135911947,1.4251774368

B3LYP/6-31G*
E(RB+HF-LYP) = -604.124842460

Zero-point correction= 0.103918 (Hartree/Particle)
Thermal correction to Energy= 0.109093
Thermal correction to Enthalpy= 0.110037
Thermal correction to Gibbs Free Energy= 0.075199
Sum of electronic and ZPE= -604.020924
Sum of electronic and thermal Energies= -604.015750
Sum of electronic and thermal Enthalpies= -604.014806
Sum of electronic and thermal Free Energies= -604.049643

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.457	19.296	73.321

C,0,0.0585550847,-0.0621391058,1.3025500867
C,0,1.2792806807,0.2564610747,1.9235037837
C,0,2.626095028,0.2384379586,1.2151728647
H,0,3.3787466854,-0.1999754073,1.8722578352
B,0,0.3136888934,1.7105267118,1.7202293371
H,0,0.0275828609,-0.2627572101,0.2364579887

H,0,-0.7602336502,-0.4707556363,1.8852233232
H,0,1.3493680074,0.0427852762,2.9859288097
H,0,-0.0326859593,2.0745031994,2.8050819135
H,0,-0.7443481792,1.4551291085,1.1120203298
H,0,0.911508855,2.3986611406,0.9463586373
Cl,0,2.6662736942,-0.769491409,-0.3084353983
H,0,2.957791999,1.2290922988,0.9098764887

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.099865	E(Thermal)=	0.106000
E(QCISD(T))=	-603.044697	E(Empiric)=	-0.101400
DE(Plus)=	-0.009627	DE(2DF)=	-0.210432
E(Delta-G3)=	-0.560837	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.827128	G3 Energy=	-603.820993
G3 Enthalpy=	-603.820049	G3 Free Energy=	-603.856895

6a-10 Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.143183568

Zero-point correction= 0.103005 (Hartree/Particle)
Thermal correction to Energy= 0.109211
Thermal correction to Enthalpy= 0.110155
Thermal correction to Gibbs Free Energy= 0.073027
Sum of electronic and ZPE= -604.040179
Sum of electronic and thermal Energies= -604.033973
Sum of electronic and thermal Enthalpies= -604.033029
Sum of electronic and thermal Free Energies= -604.070156

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.531	21.936	78.142

C,0,0.0959088736,-0.3440866432,1.5278565444
C,0,1.3453154365,0.146387371,1.8838713849
C,0,2.5239846744,0.0314530403,0.9552028415
Cl,0,3.7781188012,1.3120428434,1.24208623
B,0,0.1920088486,1.5192030928,1.5151576027
H,0,-0.0898981897,-0.7270602066,0.5292223771
H,0,-0.6254926486,-0.626201068,2.2860233958
H,0,1.5857955724,0.2407757425,2.9377720621
H,0,0.0421179232,2.0493967918,2.5758454805

H,0,-0.9072183542,1.2036657524,1.0818386843
H,0,0.7667606361,2.0436818301,0.6073910834
H,0,3.0394728653,-0.9185210256,1.1180806718
H,0,2.2230875613,0.106187479,-0.0903313584

B3LYP/6-31G*
E(RB+HF-LYP) = -604.122911986

Zero-point correction= 0.103709 (Hartree/Particle)
Thermal correction to Energy= 0.108942
Thermal correction to Enthalpy= 0.109886
Thermal correction to Gibbs Free Energy= 0.074891
Sum of electronic and ZPE= -604.019203
Sum of electronic and thermal Energies= -604.013970
Sum of electronic and thermal Enthalpies= -604.013026
Sum of electronic and thermal Free Energies= -604.048021

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	68.362	19.394	73.655

C,0,-0.0398313872,0.2461943128,0.9961326158
B,0,0.5478330696,1.5772736574,2.1238603146
C,0,1.159623572,-0.0104776081,1.6848244814
C,0,2.4932915659,-0.0406486869,0.9427607487
H,0,-0.0248223913,0.5226973265,-0.0553108531
H,0,-0.9816010475,-0.1560518606,1.3552081816
H,0,1.1059577437,-0.6477609892,2.5603185924
H,0,0.171356719,1.5310907514,3.2568328292
H,0,-0.468633514,1.8544092302,1.4574700933
H,0,1.3547889833,2.3601300584,1.715133273
H,0,2.9554183546,0.9421780988,0.8667531521
Cl,0,3.6903240344,-1.0973431,1.8058388609
H,0,2.3893242976,-0.4655911906,-0.0588122898

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.099604	E(Thermal)=	0.105910
E(QCISD(T))=	-603.044821	E(Empiric)=	-0.101400
DE(Plus)=	-0.009953	DE(2DF)=	-0.209846
E(Delta-G3)=	-0.560391	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.826807	G3 Energy=	-603.820502
G3 Enthalpy=	-603.819558	G3 Free Energy=	-603.856840

6a-11 Variational Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -604.134024592
Zero-point correction= 0.098935 (Hartree/Particle)
Thermal correction to Energy= 0.107523
Thermal correction to Enthalpy= 0.108468
Thermal correction to Gibbs Free Energy= 0.063475
Sum of electronic and zero-point Energies= -604.035090
Sum of electronic and thermal Energies= -604.026501
Sum of electronic and thermal Enthalpies= -604.025557
Sum of electronic and thermal Free Energies= -604.070550

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.472	25.823	94.695

B3LYP/6-31G*
E(RB+HF-LYP) = -604.116251192

Zero-point correction= 0.099351 (Hartree/Particle)
Thermal correction to Energy= 0.107146
Thermal correction to Enthalpy= 0.108090
Thermal correction to Gibbs Free Energy= 0.065219
Sum of electronic and ZPE= -604.016900
Sum of electronic and thermal Energies= -604.009105
Sum of electronic and thermal Enthalpies= -604.008161
Sum of electronic and thermal Free Energies= -604.051032

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	67.235	23.801	90.229

C,0,-0.64282,1.89348,0.12548
C,0,-0.21834,0.74446,-0.40662
C,0,0.30473,-0.39597,0.40368
Cl,0,2.03337,-0.80354,-0.04723
B,0,-3.61369,-0.64165,-0.05572
H,0,0.306,-0.17168,1.47165
H,0,-0.60682,2.07607,1.19751
H,0,-1.03839,2.69452,-0.49195
H,0,-0.24769,0.59259,-1.48422
H,0,-2.84445,-1.54877,-0.16644
H,0,-4.10875,-0.16002,-1.02882
H,0,-3.90173,-0.2343,1.02852

H,0,-0.25811,-1.31508,0.2275

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.095377	E(Thermal)=	0.103318
E(QCISD(T))=	-603.034085	E(Empiric)=	-0.101400
DE(Plus)=	-0.011376	DE(2DF)=	-0.206312
E(Delta-G3)=	-0.560042	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.817838	G3 Energy=	-603.809897
G3 Enthalpy=	-603.808953	G3 Free Energy=	-603.852176

6a-12 Variational Transition State

temp_allylclin_118_VTS
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.131834855
Zero-point correction= 0.098514 (Hartree/Particle)
Thermal correction to Energy= 0.107250
Thermal correction to Enthalpy= 0.108194
Thermal correction to Gibbs Free Energy= 0.061684
Sum of electronic and zero-point Energies= -604.033320
Sum of electronic and thermal Energies= -604.024585
Sum of electronic and thermal Enthalpies= -604.023641
Sum of electronic and thermal Free Energies= -604.070151

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.300	25.868	97.889

B3LYP/6-31G*
E(RB+HF-LYP) = -604.113538987

Zero-point correction= 0.098920 (Hartree/Particle)
Thermal correction to Energy= 0.106879
Thermal correction to Enthalpy= 0.107823
Thermal correction to Gibbs Free Energy= 0.063653
Sum of electronic and ZPE= -604.014619
Sum of electronic and thermal Energies= -604.006660
Sum of electronic and thermal Enthalpies= -604.005716
Sum of electronic and thermal Free Energies= -604.049886

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	67.067	23.852	92.963

C,0,0.16938,1.58576,-0.77635
C,0,-0.05691,1.2154,0.48241
C,0,-0.81421,0.01313,0.96643
H,0,-1.67535,0.31526,1.57067
B,0,3.75741,-0.50218,-0.02797
Cl,0,-1.46683,-1.0556,-0.34329
H,0,-0.19881,1.00837,-1.61903
H,0,0.72947,2.48876,-0.99849
H,0,0.32529,1.82529,1.30288
H,0,3.46608,-0.4564,1.12944
H,0,4.29868,0.42918,-0.54243
H,0,3.52042,-1.48335,-0.66446
H,0,-0.17722,-0.6223,1.58925

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.094963	E(Thermal)=	0.103063
E(QCISD(T))=	-603.031643	E(Empiric)=	-0.101400
DE(Plus)=	-0.011006	DE(2DF)=	-0.206265
E(Delta-G3)=	-0.561091	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.816442	G3 Energy=	-603.808341
G3 Enthalpy=	-603.807397	G3 Free Energy=	-603.851920

6a-13 Variational Transition State
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.134066460

Zero-point correction= 0.098902 (Hartree/Particle)
Thermal correction to Energy= 0.107522
Thermal correction to Enthalpy= 0.108466
Thermal correction to Gibbs Free Energy= 0.062739
Sum of electronic and zero-point Energies= -604.035164
Sum of electronic and thermal Energies= -604.026545
Sum of electronic and thermal Enthalpies= -604.025600
B3LYP/6-31G*
E(RB+HF-LYP) = -604.116359057

Zero-point correction= 0.099286 (Hartree/Particle)
Thermal correction to Energy= 0.107134
Thermal correction to Enthalpy= 0.108078
Thermal correction to Gibbs Free Energy= 0.064480
Sum of electronic and ZPE= -604.017073

Sum of electronic and thermal Energies= -604.009225
Sum of electronic and thermal Enthalpies= -604.008281
Sum of electronic and thermal Free Energies= -604.051879

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	67.228	23.789	91.760

C,0,0.60989,1.96567,-0.19339
C,0,-0.22573,1.1616,0.46879
C,0,-1.34065,0.41377,-0.18417
H,0,-2.30752,0.63801,0.2727
B,0,3.25327,-0.35922,-0.00891
H,0,-1.39233,0.60902,-1.2565
H,0,0.53723,2.1059,-1.2694
H,0,1.38844,2.52385,0.31934
H,0,-0.1307,1.03501,1.54591
H,0,3.42656,0.06118,1.09553
H,0,3.52468,0.32097,-0.95262
H,0,2.84185,-1.46715,-0.16932
Cl,0,-1.12878,-1.39496,0.00839

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.095315	E(Thermal)=	0.103307
E(QCISD(T))=	-603.034313	E(Empiric)=	-0.101400
DE(Plus)=	-0.011249	DE(2DF)=	-0.206384
E(Delta-G3)=	-0.560143	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.818174	G3 Energy=	-603.810182
G3 Enthalpy=	-603.809238	G3 Free Energy=	-603.853188

6a-14 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.184119965

Zero-point correction= 0.104733 (Hartree/Particle)
Thermal correction to Energy= 0.111930
Thermal correction to Enthalpy= 0.112874
Thermal correction to Gibbs Free Energy= 0.072591
Sum of electronic and ZPE= -604.079387
Sum of electronic and thermal Energies= -604.072190
Sum of electronic and thermal Enthalpies= -604.071246

Sum of electronic and thermal Free Energies= -604.111529

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.237	23.418	84.783

C,0,-0.1401026361,-0.3591615476,-0.0805628966
H,0,-0.2000750887,-1.3698688266,0.3289437622
C,0,-0.229965119,0.6988677619,1.0108880598
C,0,0.9215086564,0.574632832,2.0238133136
B,0,0.9892538229,1.6261284094,3.1783966888
Cl,0,-1.5049186592,-0.2209505679,-1.2808443875
H,0,-1.1928955458,0.6035699149,1.5255744937
H,0,1.8997161394,0.6452906384,1.5106648219
H,0,0.9498172925,-0.4332654264,2.4715432547
H,0,1.825714328,1.5121326989,4.0265578831
H,0,-0.2193890865,1.6941017463,0.55230955
H,0,0.2413686507,2.5596371931,3.2329943672
H,0,0.7812872455,-0.2664738264,-0.659768911

B3LYP/6-31G*
E(RB+HF-LYP) = -604.167910718

Zero-point correction= 0.105503 (Hartree/Particle)
Thermal correction to Energy= 0.112610
Thermal correction to Enthalpy= 0.113555
Thermal correction to Gibbs Free Energy= 0.073920
Sum of electronic and ZPE= -604.062407
Sum of electronic and thermal Energies= -604.055300
Sum of electronic and thermal Enthalpies= -604.054356
Sum of electronic and thermal Free Energies= -604.093991

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.664	23.267	83.419

C,0,-0.1381687419,-0.355702464,-0.0823316415
H,0,-0.1824690322,-1.3715615872,0.317722895
C,0,-0.238750102,0.6900834627,1.0202859776
C,0,0.9154904443,0.5662141027,2.0300726997
B,0,0.9925584664,1.6292181918,3.1745552263
Cl,0,-1.506520104,-0.221157716,-1.2765658669
H,0,-1.2007062678,0.5777897553,1.5341273482
H,0,1.889968356,0.6568652321,1.5095704201

H,0,0.9571931451,-0.4460495283,2.464252602
H,0,1.7862307751,1.4852251615,4.0597509608
H,0,-0.2400397727,1.6906132191,0.5726060402
H,0,0.304082175,2.6097923515,3.1774955196
H,0,0.7824506588,-0.2466891812,-0.6610321809

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101283	E(Thermal)=	0.108555
E(QCISD(T))=	-603.085281	E(Empiric)=	-0.101400
DE(Plus)=	-0.008900	DE(2DF)=	-0.208495
E(Delta-G3)=	-0.560813	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.863606	G3 Energy=	-603.856334
G3 Enthalpy=	-603.855390	G3 Free Energy=	-603.895368

6a-15 Product
B3LYP/6-31G**
E(RB+HF-LYP) = -604.183464886

Zero-point correction= 0.104961 (Hartree/Particle)
Thermal correction to Energy= 0.111856
Thermal correction to Enthalpy= 0.112800
Thermal correction to Gibbs Free Energy= 0.073790
Sum of electronic and ZPE= -604.078503
Sum of electronic and thermal Energies= -604.071609
Sum of electronic and thermal Enthalpies= -604.070665
Sum of electronic and thermal Free Energies= -604.109675

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.191	23.245	82.104

C,0,-0.0638090423,0.0567754288,-0.1030342452
H,0,-0.9187171362,-0.1105034062,-0.7596093089
C,0,-0.4612978091,-0.0193012314,1.3652768579
B,0,1.29532252,1.7227557371,2.3613087217
C,0,0.6757682244,0.2899357292,2.3530211815
Cl,0,1.162092691,-1.2202240111,-0.5616345064
H,0,-0.8938319182,-1.0071886612,1.5638567344
H,0,1.4878120583,-0.4466674551,2.2477204179
H,0,0.3260814569,0.119842681,3.3877233835
H,0,2.2044036581,1.9662254787,3.100240598
H,0,-1.2729252712,0.71058459,1.498654081

H,0,0.8751523571,2.6097323162,1.6720479449
H,0,0.397119211,1.0145638039,-0.3524618603

B3LYP/6-31G*
E(RB+HF-LYP) = -604.168186671

Zero-point correction= 0.105695 (Hartree/Particle)
Thermal correction to Energy= 0.112523
Thermal correction to Enthalpy= 0.113467
Thermal correction to Gibbs Free Energy= 0.074716
Sum of electronic and ZPE= -604.062492
Sum of electronic and thermal Energies= -604.055663
Sum of electronic and thermal Enthalpies= -604.054719
Sum of electronic and thermal Free Energies= -604.093470

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.610	23.101	81.560

C,0,-0.2094891298,-0.4888602949,-0.0955975832
H,0,-1.1620708842,-0.5579761547,-0.6244211124
C,0,-0.2768300555,0.5039956973,1.0588829152
B,0,1.0296303723,1.6167541179,3.0791415675
C,0,1.0477535502,0.7202291804,1.8034081735
Cl,0,0.1664764889,-2.1832832407,0.4686138623
H,0,-1.0575219441,0.1891980524,1.7614214471
H,0,1.8473989849,1.0219615479,1.1098290332
H,0,1.4035101186,-0.2532374114,2.1991619144
H,0,0.0068389351,1.882339322,3.6457587405
H,0,-0.617917577,1.4564488693,0.6267473945
H,0,2.0587719144,2.0091085271,3.5493912176
H,0,0.5766192261,-0.2301482127,-0.8092275701

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101467	E(Thermal)=	0.108469
E(QCISD(T))=	-603.085465	E(Empiric)=	-0.101400
DE(Plus)=	-0.009088	DE(2DF)=	-0.208968
E(Delta-G3)=	-0.560753	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.864206	G3 Energy=	-603.857204
G3 Enthalpy=	-603.856260	G3 Free Energy=	-603.895352

6a-16 Product
B3LYP/6-31+G**
E(RB+HF-LYP) = -604.181435096

Zero-point correction= 0.104919 (Hartree/Particle)
Thermal correction to Energy= 0.111752
Thermal correction to Enthalpy= 0.112696
Thermal correction to Gibbs Free Energy= 0.074346
Sum of electronic and ZPE= -604.076516
Sum of electronic and thermal Energies= -604.069683
Sum of electronic and thermal Enthalpies= -604.068739
Sum of electronic and thermal Free Energies= -604.107089

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.126	23.600	80.715

C,0,-0.1565269928,-0.0541918516,1.0860482605
C,0,1.0520400662,0.5822426248,1.7969194585
B,0,0.9159079361,2.0949435866,2.1873661063
C,0,2.391138575,0.2077648744,1.1627523191
H,0,2.4859533588,-0.8648217889,0.9795209696
H,0,3.2340976237,0.5511624835,1.7637158128
H,0,-0.264098149,0.3420226573,0.0716825034
H,0,-0.0518048304,-1.1429592183,1.0068986276
H,0,1.10027539,0.1493762012,2.8240037037
H,0,-0.1628576305,2.5795805305,2.364210143
H,0,-1.0827310372,0.1598370653,1.6275779338
H,0,1.8901630773,2.7505263919,2.41277672
Cl,0,2.6061146128,0.9969484433,-0.4760585581

B3LYP/6-31G*
E(RB+HF-LYP) = -604.165519263

Zero-point correction= 0.105602 (Hartree/Particle)
Thermal correction to Energy= 0.112437
Thermal correction to Enthalpy= 0.113381
Thermal correction to Gibbs Free Energy= 0.075004
Sum of electronic and ZPE= -604.059917
Sum of electronic and thermal Energies= -604.053083
Sum of electronic and thermal Enthalpies= -604.052139
Sum of electronic and thermal Free Energies= -604.090516

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 70.555 23.480 80.771

C,0,-0.1552941965,-0.0549838769,1.0889930595
C,0,1.0519675896,0.5776534372,1.8038648698
B,0,0.9170479034,2.0948175303,2.1839634955
C,0,2.3897414488,0.208538902,1.1625928197
H,0,2.4855780252,-0.86369644,0.9743286817
H,0,3.2344222505,0.5479614576,1.7644080512
H,0,-0.2585056694,0.342124734,0.0740395304
H,0,-0.0529863557,-1.1445762884,1.0098087436
H,0,1.1018696672,0.1370705255,2.8268878274
H,0,-0.1617217093,2.5869372524,2.3464253282
H,0,-1.0832099314,0.1613896496,1.6278971491
H,0,1.8918707289,2.749842618,2.4138350999
Cl,0,2.5968922488,1.0093524989,-0.4696306558

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101378	E(Thermal)=	0.108393
E(QCISD(T))=	-603.084288	E(Empiric)=	-0.101400
DE(Plus)=	-0.009311	DE(2DF)=	-0.209709
E(Delta-G3)=	-0.560285	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.863614	G3 Energy=	-603.856600
G3 Enthalpy=	-603.855656	G3 Free Energy=	-603.894380

For Anharmonic Corrections of 6a-16

Zero-point vibrational energy 273120.7 (Joules/Mol)
65.27741 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 154.77 302.37 368.36 512.52 734.59
(Kelvin) 820.08 992.66 1050.71 1134.28 1265.47
1357.99 1425.56 1481.43 1533.70 1590.44
1651.91 1674.80 1708.57 1760.63 1865.61
1931.07 2082.74 2170.69 2262.25 3431.55
3708.27 3856.92 4450.90 4544.58 4570.91
4586.90 4714.46

Zero-point correction= 0.104026 (Hartree/Particle)
Thermal correction to Energy= 0.109986
Thermal correction to Enthalpy= 0.110930
Thermal correction to Gibbs Free Energy= 0.074390
Sum of electronic and zero-point Energies= -604.022676

Sum of electronic and thermal Energies= -604.016716
Sum of electronic and thermal Enthalpies= -604.015772
Sum of electronic and thermal Free Energies= -604.052313

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.017	21.328	76.906

ZPE(harm) = 0.27079D+03 kJ/mol ZPE(anh)= 0.26608D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.33093D-46	0.23687D-45	
QZvib	0.91127D+01	0.97503D+01	
Energy	0.28644D+03	0.28197D+03	kJ/mol
Enthalpy	0.28891D+03	0.28445D+03	kJ/mol
Entropy	0.33009D+03	0.33148D+03	J/(mol K)
Sp.Heat(V)	0.89234D+02	0.91477D+02	J/(mol K)
Sp.Heat(P)	0.97549D+02	0.99792D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.33093D-46	0.23687D-45	
QZvib	0.91127D+01	0.97503D+01	
Energy	0.28644D+03	0.28197D+03	kJ/mol
Enthalpy	0.28891D+03	0.28445D+03	kJ/mol
Entropy	0.33009D+03	0.33148D+03	J/(mol K)
Sp.Heat(V)	0.89234D+02	0.91477D+02	J/(mol K)
Sp.Heat(P)	0.97549D+02	0.99792D+02	J/(mol K)

6a-17 Product

B3LYP/6-31G**
E(RB+HF-LYP) = -604.181238009
Zero-point correction= 0.105196 (Hartree/Particle)
Thermal correction to Energy= 0.112211
Thermal correction to Enthalpy= 0.113156
Thermal correction to Gibbs Free Energy= 0.074371
Sum of electronic and zero-point Energies= -604.076042
Sum of electronic and thermal Energies= -604.069027
Sum of electronic and thermal Enthalpies= -604.068082
Sum of electronic and thermal Free Energies= -604.106867

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.414	23.706	81.630

C,0,-0.1649127543,0.0722473568,1.0249790245
C,0,1.0798149974,0.5133086115,1.8532964803
B,0,0.8677142394,2.0446597516,2.1355320895
C,0,2.3510061264,0.1769446038,1.0813333781
H,0,2.4556797128,-0.8928686484,0.8863256078
Cl,0,3.8421691888,0.6534289572,2.0254468387
H,0,-0.239647039,0.6171765169,0.0767101362
H,0,-0.1084478874,-0.9967362054,0.7881671701
H,0,1.0714579296,-0.0637433068,2.7871584844
H,0,0.1648727358,2.4008542563,3.034912796
H,0,-1.0916943128,0.2377015131,1.5834836033
H,0,1.3207280832,2.8661728377,1.3928206944
H,0,2.40893098,0.7232857558,0.1372476966

B3LYP/6-31G*
E(RB+HF-LYP) = -604.165548413

Zero-point correction= 0.105908 (Hartree/Particle)
Thermal correction to Energy= 0.112906
Thermal correction to Enthalpy= 0.113850
Thermal correction to Gibbs Free Energy= 0.075089
Sum of electronic and ZPE= -604.059641
Sum of electronic and thermal Energies= -604.052643
Sum of electronic and thermal Enthalpies= -604.051698
Sum of electronic and thermal Free Energies= -604.090459

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	70.849	23.576	81.579

C,0,-0.1642206834,0.0716634988,1.0213878292
C,0,1.0768166085,0.5106588483,1.8541825588
B,0,0.8702675266,2.0432919828,2.1370181693
C,0,2.3503200996,0.1772411914,1.0845046699
H,0,2.4585446831,-0.8927603179,0.8889903575
Cl,0,3.8355010353,0.6621047011,2.0312680574
H,0,-0.2336530007,0.6172140482,0.0725471751
H,0,-0.1097783514,-0.9980252838,0.7847840202
H,0,1.0674572974,-0.0693754705,2.7862001513
H,0,0.1897445367,2.4051079031,3.0523460727

H,0,-1.0935308988,0.2404528119,1.575903701
H,0,1.3037372806,2.8631081056,1.3794691116
H,0,2.4064658666,0.7217499809,0.1388121261

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101671	E(Thermal)=	0.108845
E(QCISD(T))=	-603.084517	E(Empiric)=	-0.101400
DE(Plus)=	-0.009126	DE(2DF)=	-0.209376
E(Delta-G3)=	-0.560185	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.862933	G3 Energy=	-603.855759
G3 Enthalpy=	-603.854815	G3 Free Energy=	-603.893925

6a-18 Product
B3LYP/6-31G*
E(RB+HF-LYP) = -604.160289528

Zero-point correction= 0.106245 (Hartree/Particle)
Thermal correction to Energy= 0.112398
Thermal correction to Enthalpy= 0.113342
Thermal correction to Gibbs Free Energy= 0.076139
Sum of electronic and ZPE= -604.054045
Sum of electronic and thermal Energies= -604.047891
Sum of electronic and thermal Enthalpies= -604.046947
Sum of electronic and thermal Free Energies= -604.160289528

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	70.531	21.262	78.301

C,0,-0.0780747074,0.2034671464,1.1076771743
C,0,1.2354298304,0.4787451558,1.9184050071
C,0,2.5085081651,0.2155021586,1.1182730693
H,0,3.4002476969,0.4431887521,1.7043047386
B,0,0.7740842594,1.9387426583,2.1173916839
H,0,0.060527227,0.4244966866,0.0452018301
H,0,-0.3486332205,-0.8530443598,1.1980459519
H,0,1.2191551624,-0.1287013807,2.8274904898
H,0,-0.0706749371,2.0675178179,2.9329369706
H,0,-0.9490715376,0.7739809673,1.4577380158
H,0,1.0583609849,2.8235790701,1.364722375
Cl,0,2.6908707313,-1.5401730089,0.6221436182
H,0,2.5308943452,0.7931763363,0.1918950755

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101672	E(Thermal)=	0.108832
E(QCISD(T))=	-603.084361	E(Empiric)=	-0.101400
DE(Plus)=	-0.009129	DE(2DF)=	-0.209442
E(Delta-G3)=	-0.560313	E(G3-Empiric)=	-0.101400
G3(0 K)=	-603.862972	G3 Energy=	-603.855812
G3 Enthalpy=	-603.854868	G3 Free Energy=	-603.893920

6b-1 Starting Material
B3LYP/6-31+G**
E(RB3LYP) = -694.268726639

Zero-point correction= 0.136869 (Hartree/Particle)
Thermal correction to Energy= 0.143497
Thermal correction to Enthalpy= 0.144441
Thermal correction to Gibbs Free Energy= 0.105887
Sum of electronic and ZPE= -694.131858
Sum of electronic and thermal Energies= -694.125230
Sum of electronic and thermal Enthalpies= -694.124285
Sum of electronic and thermal Free Energies= -694.162839

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	90.046	25.243	81.143

C,0,2.19137,0.56255,1.225893
C,0,2.540926,-0.659165,2.044404
C,0,1.90068,-0.962318,3.17667
C,0,0.758176,-0.180317,3.767322
C,0,0.191,0.826636,2.750251
C,0,1.315102,1.556568,2.003782
H,0,1.108815,0.336332,4.67233
H,0,3.343118,-1.300814,1.689775
H,0,1.6775,0.244757,0.305613
H,0,-0.024411,-0.873203,4.097705
H,0,-0.436046,0.291015,2.025015
H,0,-0.460772,1.540311,3.266816
H,0,1.937911,2.097855,2.7288
H,0,0.899966,2.305843,1.320136
H,0,3.117161,1.050426,0.894632
Cl,0,2.391825,-2.380202,4.121883

B3LYP/6-31G*
E(RB3LYP) = -694.248525457

Zero-point correction= 0.137773 (Hartree/Particle)
Thermal correction to Energy= 0.144375
Thermal correction to Enthalpy= 0.145319
Thermal correction to Gibbs Free Energy= 0.106802
Sum of electronic and ZPE= -694.110753
Sum of electronic and thermal Energies= -694.104151
Sum of electronic and thermal Enthalpies= -694.103206
Sum of electronic and thermal Free Energies= -694.141723

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	90.597	25.054	81.065

C,0,2.1912409159,0.5619366371,1.2264860178
C,0,2.5398272793,-0.6592704841,2.0451286176
C,0,1.9004954102,-0.9620821925,3.1759650939
C,0,0.7588954434,-0.1796293613,3.7676714867
C,0,0.1912222549,0.8257286304,2.7497778858
C,0,1.3152974826,1.5558367665,2.0044277401
H,0,1.1091557488,0.3389908204,4.6721723363
H,0,3.342922172,-1.2997201463,1.6895883858
H,0,1.6774321739,0.2452762433,0.3051230141
H,0,-0.0246116429,-0.8712051819,4.1004209401
H,0,-0.4346581688,0.2888003219,2.0241699483
H,0,-0.4621808753,1.5394407555,3.2652108001
H,0,1.9382282253,2.0963534372,2.7301864842
H,0,0.9006246739,2.3061548401,1.3209180109
H,0,3.117105883,1.0507369866,0.8944610054
Cl,0,2.391324024,-2.3810740729,4.1193192329

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.132262	E(Thermal)=	0.139086
E(QCISD(T))=	-692.930565	E(Empiric)=	-0.135200
DE(Plus)=	-0.013931	DE(2DF)=	-0.269463
E(Delta-G3)=	-0.673948	E(G3-Empiric)=	-0.135200
G3(0 K)=	-693.890846	G3 Energy=	-693.884021
G3 Enthalpy=	-693.883077	G3 Free Energy=	-693.921975

For Anharmonic Corrections of 6b-1

Zero-point vibrational energy 361721.2 (Joules/Mol)
86.45344 (Kcal/Mol)
Warning -- explicit consideration of 8 degrees of freedom as vibrations may cause significant error
Vibrational temperatures: 174.94 329.86 407.61 437.01 533.92
(Kelvin) 618.81 706.39 798.87 1066.54 1184.75
1223.86 1236.81 1334.11 1360.34 1371.18
1473.69 1534.69 1575.38 1596.97 1690.51
1734.55 1840.18 1873.88 1919.01 1985.47
1994.55 2011.91 2022.62 2163.23 2174.37
2186.29 2202.30 2493.45 4331.48 4359.27
4370.23 4378.21 4400.04 4428.33 4440.64
4448.24 4595.53

Zero-point correction= 0.137772 (Hartree/Particle)
Thermal correction to Energy= 0.144375
Thermal correction to Enthalpy= 0.145319
Thermal correction to Gibbs Free Energy= 0.106802
Sum of electronic and zero-point Energies= -694.110753
Sum of electronic and thermal Energies= -694.104151
Sum of electronic and thermal Enthalpies= -694.103207
Sum of electronic and thermal Free Energies= -694.141723

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.596	25.054	81.065

ZPE(harm) = 0.36172D+03 kJ/mol ZPE(anh)= 0.35674D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.47457D-62	0.37086D-61	
QZvib	0.11144D+02	0.11686D+02	
Energy	0.37906D+03	0.37428D+03	kJ/mol
Enthalpy	0.38153D+03	0.37675D+03	kJ/mol
Entropy	0.33918D+03	0.34024D+03	J/(mol K)
Sp.Heat(V)	0.10483D+03	0.10672D+03	J/(mol K)
Sp.Heat(P)	0.11314D+03	0.11503D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.47457D-62	0.37086D-61	
QZvib	0.11144D+02	0.11686D+02	
Energy	0.37906D+03	0.37428D+03	kJ/mol
Enthalpy	0.38153D+03	0.37675D+03	kJ/mol
Entropy	0.33918D+03	0.34024D+03	J/(mol K)
Sp.Heat(V)	0.10483D+03	0.10672D+03	J/(mol K)
Sp.Heat(P)	0.11314D+03	0.11503D+03	J/(mol K)

6b-2 Complex
B3LYP/6-31+G**
E(RB3LYP) = -720.891733422

Zero-point correction= 0.167788 (Hartree/Particle)
Thermal correction to Energy= 0.177200
Thermal correction to Enthalpy= 0.178144
Thermal correction to Gibbs Free Energy= 0.133600
Sum of electronic and ZPE= -720.723946
Sum of electronic and thermal Energies= -720.714533
Sum of electronic and thermal Enthalpies= -720.713589
Sum of electronic and thermal Free Energies= -720.758133

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.195	35.004	93.751

C,0,0.6422298116,1.4403852462,-0.5058546203
C,0,-0.0314845407,0.1316688705,-0.0730106154
C,0,0.1783738543,-0.1357529695,1.4271070715
C,0,1.5880439874,0.1805470112,1.8898198163
C,0,2.4816281536,0.8125223151,1.0916954462
C,0,2.159447675,1.3755790008,-0.2670964436
H,0,1.9335837142,-0.2817956286,2.8087595931
B,0,1.6503244146,2.3134613976,2.7737533761
Cl,0,4.1947933431,0.8181202926,1.5022482025
H,0,0.4634967265,2.2481084255,2.8969987599
H,0,2.0763097374,3.092145214,1.9715032453
H,0,-0.0117860326,-1.1933318587,1.650851095
H,0,-0.5409127853,0.434053463,2.0258788518
H,0,2.6195397852,2.3636116941,-0.368261414
H,0,2.6404855217,0.7295669492,-1.0151537061

H,0,0.453826679,1.6410279304,-1.5662917857
H,0,0.2213756963,2.2797474634,0.0600227791
H,0,-1.1033957545,0.1570257229,-0.29716769
H,0,0.3930126306,-0.6981235186,-0.6543363313
H,0,2.3606293826,2.0013559789,3.6805303695

B3LYP/6-31G*
E(RB3LYP) = -720.868913189

Zero-point correction= 0.168921 (Hartree/Particle)
Thermal correction to Energy= 0.178264
Thermal correction to Enthalpy= 0.179208
Thermal correction to Gibbs Free Energy= 0.134853
Sum of electronic and ZPE= -720.699992
Sum of electronic and thermal Energies= -720.690649
Sum of electronic and thermal Enthalpies= -720.689705
Sum of electronic and thermal Free Energies= -720.734061

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.863	34.749	93.355

C,0,0.6432789021,1.4422700423,-0.5015618841
C,0,-0.0311071042,0.1335238867,-0.0716338204
C,0,0.1790091977,-0.1373575739,1.427651121
C,0,1.5885539627,0.1791387561,1.8907493875
C,0,2.4817414183,0.8129489899,1.0949318778
C,0,2.1603217022,1.3746138621,-0.2649054645
H,0,1.9327040355,-0.2837443286,2.8101858346
B,0,1.6494716025,2.3113869628,2.7640117349
Cl,0,4.1945533399,0.8195990296,1.5070089941
H,0,0.4614850479,2.2449793782,2.8895683401
H,0,2.0720083863,3.0951646976,1.962625186
H,0,-0.0118309786,-1.1959825503,1.6487878167
H,0,-0.5401009655,0.430996242,2.0283377456
H,0,2.6221971113,2.361851005,-0.368584392
H,0,2.6387643889,0.7266866286,-1.0136145263
H,0,0.4533039085,1.6467354427,-1.561499983
H,0,0.2249969786,2.2807819078,0.068126796
H,0,-1.1034876781,0.159679417,-0.2956283228
H,0,0.3928336835,-0.6955548551,-0.6548990973
H,0,2.3608250605,2.0022060596,3.672338656

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162164	E(Thermal)=	0.171807
E(QCISD(T))=	-719.425833	E(Empiric)=	-0.155480
DE(Plus)=	-0.015286	DE(2DF)=	-0.311438
E(Delta-G3)=	-0.723363	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.469236	G3 Energy=	-720.459593
G3 Enthalpy=	-720.458649	G3 Free Energy=	-720.503576

For Anharmonic Corrections of 6b-2

Zero-point vibrational energy 443501.1 (Joules/Mol)
105.99931 (Kcal/Mol)
Warning -- explicit consideration of 12 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 142.04 181.81 183.12 240.64 286.51
(Kelvin) 408.44 418.53 456.08 539.44 632.58
704.85 804.74 1008.35 1020.72 1074.96
1195.77 1222.66 1268.25 1330.95 1365.27
1374.57 1476.85 1537.73 1577.49 1595.05
1602.20 1699.39 1710.12 1721.01 1737.77
1847.22 1878.94 1920.46 1988.98 1996.93
2012.39 2022.12 2152.25 2169.86 2190.59
2206.49 2386.94 3696.29 3837.99 3875.54
4368.97 4370.90 4388.38 4402.97 4436.55
4454.98 4461.45 4470.62 4626.02

Zero-point correction=	0.168921 (Hartree/Particle)
Thermal correction to Energy=	0.178264
Thermal correction to Enthalpy=	0.179209
Thermal correction to Gibbs Free Energy=	0.134851
Sum of electronic and zero-point Energies=	-720.699993
Sum of electronic and thermal Energies=	-720.690649
Sum of electronic and thermal Enthalpies=	-720.689705
Sum of electronic and thermal Free Energies=	-720.734062

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.863	34.750	93.358

ZPE(harm) = 0.44350D+03 kJ/mol ZPE(anh)= 0.43514D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00
Harmonic value SPT anharmonic value

Qvib	0.33885D-75	0.52588D-73	
QZvib	0.16902D+03	0.89955D+03	
Energy	0.46803D+03	0.45979D+03	kJ/mol
Enthalpy	0.47051D+03	0.46227D+03	kJ/mol
Entropy	0.39061D+03	0.41322D+03	J/(mol K)
Sp.Heat(V)	0.14539D+03	0.14341D+03	J/(mol K)
Sp.Heat(P)	0.15371D+03	0.15173D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.33885D-75	0.52588D-73	
QZvib	0.16902D+03	0.89955D+03	
Energy	0.46803D+03	0.45979D+03	kJ/mol
Enthalpy	0.47051D+03	0.46227D+03	kJ/mol
Entropy	0.39061D+03	0.41322D+03	J/(mol K)
Sp.Heat(V)	0.14539D+03	0.14341D+03	J/(mol K)
Sp.Heat(P)	0.15371D+03	0.15173D+03	J/(mol K)

6b-3 Complex
B3LYP/6-31+G**
E(RB3LYP) = -720.891693942

Zero-point correction= 0.167710 (Hartree/Particle)
Thermal correction to Energy= 0.177137
Thermal correction to Enthalpy= 0.178082
Thermal correction to Gibbs Free Energy= 0.133474
Sum of electronic and ZPE= -720.723984
Sum of electronic and thermal Energies= -720.714557
Sum of electronic and thermal Enthalpies= -720.713612
Sum of electronic and thermal Free Energies= -720.758220

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.155	35.064	93.884

C,0,2.2065459785,0.5109284575,1.1780751392
C,0,2.4184311865,-0.8857052828,1.7224052632
C,0,1.8790135409,-1.2821371687,2.8993572119
C,0,1.0920635273,-0.3860630231,3.8248723844
C,0,0.6324012781,0.9019795592,3.1148560682
C,0,1.7472612813,1.5057639749,2.2521488733
B,0,4.2864684226,-0.7979766833,3.0656218967

H,0,1.7094092372,-0.1544857983,4.7011271544
H,0,2.8460953622,-1.6285735943,1.0567073187
H,0,1.4493491613,0.4397001521,0.3820459945
H,0,0.2276845427,-0.9461065025,4.1961868873
H,0,-0.2326854709,0.6705611246,2.4790406236
H,0,0.2884984202,1.6226732181,3.864833228
H,0,2.600838669,1.7720471128,2.8868680642
H,0,1.4019491302,2.4301099826,1.7758994446
H,0,3.1264538638,0.8574186717,0.6956286804
H,0,4.7412134816,-1.7995684413,2.6019698173
H,0,4.5408422112,0.2597381248,2.5686126937
H,0,3.9747730766,-0.8052387208,4.2190928335
Cl,0,1.9127470995,-2.9816261632,3.360985423

B3LYP/6-31G*
E(RB3LYP) = -720.868920991

Zero-point correction= 0.168862 (Hartree/Particle)
Thermal correction to Energy= 0.178215
Thermal correction to Enthalpy= 0.179159
Thermal correction to Gibbs Free Energy= 0.134753
Sum of electronic and ZPE= -720.700059
Sum of electronic and thermal Energies= -720.690706
Sum of electronic and thermal Enthalpies= -720.689762
Sum of electronic and thermal Free Energies= -720.734168

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.831	34.790	93.460

C,0,2.2159716804,0.5150151807,1.179772613
C,0,2.4238348023,-0.8835556823,1.7204169386
C,0,1.8776448057,-1.2834941788,2.8924136642
C,0,1.0852912304,-0.3898110234,3.8165992515
C,0,0.6356002141,0.9034158684,3.1102284017
C,0,1.7582453654,1.5059081925,2.2575707194
B,0,4.269643553,-0.80084775,3.0740502516
H,0,1.6961519404,-0.1649692235,4.6992540819
H,0,2.8549090409,-1.6236984904,1.0535511105
H,0,1.4593264055,0.4496998398,0.3820643595
H,0,0.2152873028,-0.9485784835,4.1783077604
H,0,-0.2266423696,0.6788747451,2.4676102231
H,0,0.2895667553,1.6221145091,3.861798579
H,0,2.6113070549,1.761470866,2.8979081336

H,0,1.4213514634,2.4361773851,1.7857689803
H,0,3.1379029845,0.8610548798,0.7001970951
H,0,4.7238789799,-1.810462381,2.6249269238
H,0,4.5381431278,0.2505676795,2.56751995
H,0,3.9559836248,-0.7909382826,4.2285321076
Cl,0,1.9059560382,-2.9845046506,3.347843855

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162107	E(Thermal)=	0.171760
E(QCISD(T))=	-719.425759	E(Empiric)=	-0.155480
DE(Plus)=	-0.015268	DE(2DF)=	-0.311347
E(Delta-G3)=	-0.723229	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.468975	G3 Energy=	-720.459323
G3 Enthalpy=	-720.458378	G3 Free Energy=	-720.503356

For Anharnonic Corrections of 6b-3

Zero-point vibrational energy 443345.7 (Joules/Mol)
105.96217 (Kcal/Mol)
Warning -- explicit consideration of 12 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 123.51 174.29 220.69 241.73 278.36
(Kelvin) 385.50 434.85 459.94 537.22 622.73
716.59 808.41 992.09 1009.70 1068.52
1194.16 1223.64 1273.37 1324.10 1363.69
1373.72 1481.33 1529.46 1573.77 1598.56
1600.54 1692.56 1713.67 1724.09 1738.81
1847.03 1881.36 1921.28 1991.20 1993.36
2015.43 2025.24 2156.42 2167.88 2188.07
2202.95 2388.16 3697.21 3844.77 3872.85
4339.04 4375.05 4400.74 4407.43 4446.38
4450.67 4459.86 4467.76 4624.60

Zero-point correction=	0.168861 (Hartree/Particle)
Thermal correction to Energy=	0.178215
Thermal correction to Enthalpy=	0.179159
Thermal correction to Gibbs Free Energy=	0.134752
Sum of electronic and zero-point Energies=	-720.700060
Sum of electronic and thermal Energies=	-720.690706
Sum of electronic and thermal Enthalpies=	-720.689762
Sum of electronic and thermal Free Energies=	-720.734169

E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	111.831	34.790	93.463

ZPE(harm) = 0.44335D+03 kJ/mol ZPE(anh)= 0.43567D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.37463D-75	0.18370D-72	
QZvib	0.17552D+03	0.38886D+04	
Energy	0.46790D+03	0.46251D+03	kJ/mol
Enthalpy	0.47038D+03	0.46499D+03	kJ/mol
Entropy	0.39105D+03	0.42447D+03	J/(mol K)
Sp.Heat(V)	0.14556D+03	0.15186D+03	J/(mol K)
Sp.Heat(P)	0.15387D+03	0.16017D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.37463D-75	0.18370D-72	
QZvib	0.17552D+03	0.38886D+04	
Energy	0.46790D+03	0.46251D+03	kJ/mol
Enthalpy	0.47038D+03	0.46499D+03	kJ/mol
Entropy	0.39105D+03	0.42447D+03	J/(mol K)
Sp.Heat(V)	0.14556D+03	0.15186D+03	J/(mol K)
Sp.Heat(P)	0.15387D+03	0.16017D+03	J/(mol K)

6b-4 Transition State

B3LYP/6-31+G**

E(RB3LYP) = -720.886878481

Zero-point correction= 0.168640 (Hartree/Particle)
Thermal correction to Energy= 0.176429
Thermal correction to Enthalpy= 0.177373
Thermal correction to Gibbs Free Energy= 0.136545
Sum of electronic and ZPE= -720.718239
Sum of electronic and thermal Energies= -720.710450
Sum of electronic and thermal Enthalpies= -720.709506
Sum of electronic and thermal Free Energies= -720.750334

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 110.711 31.427 85.930

C,0,2.227941,0.594174,1.244309
C,0,2.722815,-0.525636,2.141942
C,0,2.083096,-0.86177,3.358513
C,0,0.81123,-0.13116,3.81527
C,0,0.224243,0.814009,2.751003
C,0,1.317826,1.578722,1.994502
B,0,3.596697,-0.083071,3.713941
H,0,1.024509,0.426691,4.73274
Cl,0,3.547352,-1.833833,1.243505
H,0,1.653092,0.106832,0.44614
H,0,0.064096,-0.888443,4.079778
H,0,-0.359914,0.231393,2.025057
H,0,-0.474445,1.512169,3.225277
H,0,1.908565,2.187662,2.687715
H,0,0.87278,2.265388,1.265592
H,0,3.072473,1.098517,0.765655
H,0,4.138582,0.218527,2.640609
H,0,3.361808,0.973039,4.222598
H,0,4.336017,-0.90131,4.172936

B3LYP/6-31G*
E(RB3LYP) = -720.863102009

Zero-point correction= 0.169742 (Hartree/Particle)
Thermal correction to Energy= 0.177474
Thermal correction to Enthalpy= 0.178419
Thermal correction to Gibbs Free Energy= 0.137668
Sum of electronic and ZPE= -720.693360
Sum of electronic and thermal Energies= -720.685628
Sum of electronic and thermal Enthalpies= -720.684683
Sum of electronic and thermal Free Energies= -720.725434

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 111.367 31.105 85.767

C,0,2.2282991842,0.5944377522,1.2446108812
C,0,2.7298023398,-0.5214047277,2.1445039532
C,0,2.0886195996,-0.8588671604,3.3644689062
C,0,0.8119095659,-0.1314284306,3.815162001
C,0,0.2261107139,0.8128563632,2.7498771084

C,0,1.3200876521,1.5787555814,1.9962464485
B,0,3.5883690364,-0.086494007,3.7227784219
H,0,1.0205529723,0.4278472678,4.7332251754
Cl,0,3.5465267408,-1.8335534915,1.2425153869
H,0,1.6498787152,0.1031607263,0.4509126062
H,0,0.0636370994,-0.8888223143,4.078251643
H,0,-0.3555327076,0.2297906455,2.0217640001
H,0,-0.4753216821,1.5102596515,3.2223439218
H,0,1.9120558969,2.1851079161,2.6913339808
H,0,0.8763050451,2.2683470584,1.2685390995
H,0,3.0690598176,1.099147679,0.7586046626
H,0,4.121784064,0.212754032,2.6364654801
H,0,3.3674934882,0.9795005587,4.2198355587
H,0,4.3427193448,-0.8980951961,4.1709333577
H,0,2.1603811135,-1.8998849045,3.6615334064
H,0,2.163975,-1.898485,3.666824

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162952	E(Thermal)=	0.170980
E(QCISD(T))=	-719.420751	E(Empiric)=	-0.155480
DE(Plus)=	-0.015426	DE(2DF)=	-0.313089
E(Delta-G3)=	-0.722444	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.464238	G3 Energy=	-720.456210
G3 Enthalpy=	-720.455266	G3 Free Energy=	-720.496518

For Anharmonic Corrections of 6b-4

Zero-point vibrational energy 445659.1 (Joules/Mol)
106.51509 (Kcal/Mol)
Warning -- explicit consideration of 11 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 165.19 267.17 376.73 424.27 457.96
(Kelvin) 516.46 622.22 688.82 726.31 792.66
872.17 1020.03 1120.38 1155.91 1203.26
1235.58 1307.59 1331.77 1375.27 1408.59
1487.34 1552.24 1575.70 1602.36 1625.71
1634.80 1699.66 1724.07 1732.46 1862.06
1884.47 1909.79 1984.22 1999.16 2001.58
2023.04 2117.84 2176.41 2187.19 2189.91
2210.09 3381.46 3709.08 3864.13 4361.50
4391.41 4398.88 4405.14 4435.99 4457.62
4465.54 4478.25 4603.39

Zero-point correction= 0.169743 (Hartree/Particle)
Thermal correction to Energy= 0.177475
Thermal correction to Enthalpy= 0.178419
Thermal correction to Gibbs Free Energy= 0.137668
Sum of electronic and zero-point Energies= -720.693359
Sum of electronic and thermal Energies= -720.685627
Sum of electronic and thermal Enthalpies= -720.684683
Sum of electronic and thermal Free Energies= -720.725434

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.367	31.105	85.767

ZPE(harm) = 0.44230D+03 kJ/mol ZPE(anh)= 0.43590D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.71570D-76	0.10918D-74	
QZvib	0.21950D+02	0.25328D+02	
Energy	0.46260D+03	0.45664D+03	kJ/mol
Enthalpy	0.46508D+03	0.45912D+03	kJ/mol
Entropy	0.36717D+03	0.36983D+03	J/(mol K)
Sp.Heat(V)	0.13015D+03	0.13319D+03	J/(mol K)
Sp.Heat(P)	0.13846D+03	0.14151D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.71570D-76	0.10918D-74	
QZvib	0.21950D+02	0.25328D+02	
Energy	0.46260D+03	0.45664D+03	kJ/mol
Enthalpy	0.46508D+03	0.45912D+03	kJ/mol
Entropy	0.36717D+03	0.36983D+03	J/(mol K)
Sp.Heat(V)	0.13015D+03	0.13319D+03	J/(mol K)
Sp.Heat(P)	0.13846D+03	0.14151D+03	J/(mol K)

6b-5 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -720.886533558

Zero-point correction= 0.168450 (Hartree/Particle)
Thermal correction to Energy= 0.176271
Thermal correction to Enthalpy= 0.177216

Thermal correction to Gibbs Free Energy= 0.136221
Sum of electronic and ZPE= -720.718084
Sum of electronic and thermal Energies= -720.710262
Sum of electronic and thermal Enthalpies= -720.709318
Sum of electronic and thermal Free Energies= -720.750313

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.612	31.426	86.281

C,0,2.4500912042,0.8526276277,1.1541112796
C,0,2.0819683586,1.4317226676,-0.2145148552
C,0,0.5568018987,1.4997447778,-0.4060542762
C,0,-0.0934790178,0.1500061467,-0.0816911946
C,0,0.1308818242,-0.214096598,1.3919199332
C,0,1.5625561311,0.0156703189,1.872508373
B,0,2.8094937339,-0.9654827047,1.1858776302
Cl,0,3.5901920666,1.8515989911,2.1074892109
H,0,1.6837101882,0.0145174092,2.9512171281
H,0,2.351989085,-1.5942119674,0.273735585
H,0,3.4317488848,-1.4263909617,2.0963207356
H,0,-0.1558128795,-1.2542718488,1.5809578445
H,0,-0.5246676262,0.4103455394,2.0162085708
H,0,2.5310911997,2.4234188284,-0.3049958412
H,0,2.5214632845,0.8084830621,-0.9995405847
H,0,0.3453719166,1.7995394247,-1.4386696233
H,0,0.1361532706,2.2785736565,0.2442440097
H,0,-1.1690471988,0.1812868302,-0.2890002654
H,0,0.3323226338,-0.6257752086,-0.7301669054
H,0,3.6360930419,-0.2250279909,0.6381782454

B3LYP/6-31+G*
E(RB3LYP) = -720.862675366

Zero-point correction= 0.169564 (Hartree/Particle)
Thermal correction to Energy= 0.177331
Thermal correction to Enthalpy= 0.178276
Thermal correction to Gibbs Free Energy= 0.137350
Sum of electronic and ZPE= -720.693111
Sum of electronic and thermal Energies= -720.685344
Sum of electronic and thermal Enthalpies= -720.684400
Sum of electronic and thermal Free Energies= -720.725326

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 111.277 31.103 86.136

C,0,2.4535362924,0.8485900395,1.1524741025
C,0,2.0829859957,1.4272704364,-0.2169283563
C,0,0.5580968417,1.4997402689,-0.4037730842
C,0,-0.0926403439,0.1505486183,-0.0803877546
C,0,0.1307004569,-0.2131011955,1.392965128
C,0,1.5652735638,0.0059117444,1.8705744217
B,0,2.8023460326,-0.9691199924,1.1896383198
Cl,0,3.5795570431,1.8601668108,2.1109255032
H,0,1.6822540763,0.0143501212,2.9501720397
H,0,2.3639391504,-1.5906656069,0.2619840286
H,0,3.4380175643,-1.4299356258,2.0919103547
H,0,-0.163746871,-1.2515134389,1.5825883853
H,0,-0.5221176464,0.4158789106,2.0163221216
H,0,2.5361168752,2.4170993838,-0.3133049531
H,0,2.5167373536,0.7996770513,-1.0021653987
H,0,0.3442706751,1.802733566,-1.4354986454
H,0,0.141013731,2.2782427755,0.2496873639
H,0,-1.168434867,0.1819226065,-0.289110812
H,0,0.3340822224,-0.6254047792,-0.7287020403
H,0,3.6269338538,-0.2101136944,0.6487642756

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162782	E(Thermal)=	0.170843
E(QCISD(T))=	-719.420217	E(Empiric)=	-0.155480
DE(Plus)=	-0.015548	DE(2DF)=	-0.312872
E(Delta-G3)=	-0.722306	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.463642	G3 Energy=	-720.455581
G3 Enthalpy=	-720.454637	G3 Free Energy=	-720.496064

For Anharmonic Corrections of 6b-5

Zero-point vibrational energy 445191.6 (Joules/Mol)
106.40334 (Kcal/Mol)
Warning -- explicit consideration of 10 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 140.79 251.41 375.94 425.59 470.63
(Kelvin) 516.18 610.67 642.48 788.95 820.39
901.71 1013.96 1067.13 1159.19 1198.63
1230.32 1324.96 1331.54 1357.04 1430.21
1480.24 1545.94 1572.13 1590.57 1632.02
1659.09 1685.83 1721.61 1724.35 1862.78

1885.83 1906.04 1985.83 1990.10 2003.85
2021.38 2123.55 2172.10 2184.42 2186.37
2205.82 3388.39 3681.70 3846.23 4350.31
4375.81 4390.71 4427.32 4438.83 4446.55
4455.06 4503.77 4586.13

Zero-point correction= 0.169565 (Hartree/Particle)
Thermal correction to Energy= 0.177332
Thermal correction to Enthalpy= 0.178276
Thermal correction to Gibbs Free Energy= 0.137350
Sum of electronic and zero-point Energies= -720.693111
Sum of electronic and thermal Energies= -720.685344
Sum of electronic and thermal Enthalpies= -720.684399
Sum of electronic and thermal Free Energies= -720.725325

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.277	31.103	86.135

ZPE(harm) = 0.44177D+03 kJ/mol ZPE(anh)= 0.43602D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.10280D-75	0.77639D-75	
QZvib	0.25470D+02	0.18941D+02	
Energy	0.46216D+03	0.45633D+03	kJ/mol
Enthalpy	0.46464D+03	0.45881D+03	kJ/mol
Entropy	0.36870D+03	0.36596D+03	J/(mol K)
Sp.Heat(V)	0.13013D+03	0.13208D+03	J/(mol K)
Sp.Heat(P)	0.13845D+03	0.14039D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.10280D-75	0.77639D-75	
QZvib	0.25470D+02	0.18941D+02	
Energy	0.46216D+03	0.45633D+03	kJ/mol
Enthalpy	0.46464D+03	0.45881D+03	kJ/mol
Entropy	0.36870D+03	0.36596D+03	J/(mol K)
Sp.Heat(V)	0.13013D+03	0.13208D+03	J/(mol K)
Sp.Heat(P)	0.13845D+03	0.14039D+03	J/(mol K)

6b-6 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -720.887023257

Zero-point correction= 0.168485 (Hartree/Particle)
Thermal correction to Energy= 0.176385
Thermal correction to Enthalpy= 0.177330
Thermal correction to Gibbs Free Energy= 0.136352
Sum of electronic and ZPE= -720.718538
Sum of electronic and thermal Energies= -720.710638
Sum of electronic and thermal Enthalpies= -720.709694
Sum of electronic and thermal Free Energies= -720.750671

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.684	31.715	86.245

C,0,2.4456869832,0.879288293,1.1659894594
C,0,2.0570216354,1.486042026,-0.1808079646
C,0,0.5339621785,1.4885398463,-0.3987075104
C,0,-0.0703953411,0.1156360338,-0.0828171222
C,0,0.1496893611,-0.2510039947,1.3941072038
C,0,1.576716443,0.0127575696,1.8578922696
Cl,0,1.7011793422,0.0290881556,3.6587222981
B,0,2.8188161116,-0.9563086562,1.0986217286
H,0,3.2005050344,1.4013433846,1.7451660129
H,0,2.3227977071,-1.5164901804,0.1655480599
H,0,3.352300158,-1.5241289704,2.0015164677
H,0,-0.1126218823,-1.29609264,1.5845573035
H,0,-0.5122036925,0.3630627604,2.0182153206
H,0,2.453885726,2.5068827877,-0.2137662775
H,0,2.5443541664,0.9347478486,-0.9910025369
H,0,0.3191636373,1.7793891393,-1.4330663981
H,0,0.070876876,2.247519317,0.2461988777
H,0,-1.1470790649,0.1146559711,-0.2871511967
H,0,0.3771903966,-0.6445857932,-0.7328628074
H,0,3.7154692238,-0.238886898,0.649706812

B3LYP/6-31G*
E(RB3LYP) = -720.863707438

Zero-point correction= 0.169620 (Hartree/Particle)
Thermal correction to Energy= 0.177463
Thermal correction to Enthalpy= 0.178407

Thermal correction to Gibbs Free Energy= 0.137518
Sum of electronic and ZPE= -720.694087
Sum of electronic and thermal Energies= -720.686244
Sum of electronic and thermal Enthalpies= -720.685300
Sum of electronic and thermal Free Energies= -720.726190

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.360	31.405	86.060

C,0,2.4479914789,0.875138506,1.1646974569
C,0,2.058073334,1.4840581699,-0.1817575942
C,0,0.5350601936,1.4881774403,-0.3970866411
C,0,-0.0688631416,0.1152505813,-0.082633
C,0,0.1487869861,-0.2499124873,1.3944338738
C,0,1.5784882626,0.0037401843,1.8564448596
Cl,0,1.700733532,0.0284856472,3.6583445901
B,0,2.811627859,-0.958792897,1.1033243532
H,0,3.1957962104,1.4036743509,1.7478257119
H,0,2.3270786033,-1.5186774073,0.1626062684
H,0,3.366058877,-1.5230604327,1.9972074002
H,0,-0.121940782,-1.2929454389,1.5865649974
H,0,-0.510345798,0.369778615,2.016618749
H,0,2.4564051241,2.5047426383,-0.2166557435
H,0,2.5427162627,0.9317484816,-0.9932001918
H,0,0.3189858251,1.7817497575,-1.4309170426
H,0,0.0733577432,2.2463365948,0.250258215
H,0,-1.1454471391,0.1132386281,-0.290103088
H,0,0.3813743079,-0.6450952215,-0.7313721992
H,0,3.7013772606,-0.2261797105,0.651459025

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162836	E(Thermal)=	0.170975
E(QCISD(T))=	-719.420998	E(Empiric)=	-0.155480
DE(Plus)=	-0.015441	DE(2DF)=	-0.312100
E(Delta-G3)=	-0.722277	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.463459	G3 Energy=	-720.455320
G3 Enthalpy=	-720.454376	G3 Free Energy=	-720.495772

For Anharmonic Corrections of 6b-6

Zero-point vibrational energy 445338.4 (Joules/Mol)
106.43843 (Kcal/Mol)
Warning -- explicit consideration of 11 degrees of freedom as

vibrations may cause significant error
Vibrational temperatures: 190.34 249.10 370.90 420.49 456.09
(Kelvin) 503.94 565.18 661.21 683.06 762.57
852.95 984.38 1093.82 1169.51 1205.36
1234.85 1322.74 1336.26 1365.47 1445.39
1499.33 1547.63 1562.33 1598.66 1618.47
1686.75 1701.15 1728.77 1745.08 1862.38
1883.42 1909.66 1988.83 1993.36 1997.88
2022.25 2125.84 2176.07 2188.44 2191.36
2208.24 3399.46 3714.64 3868.20 4374.36
4385.50 4401.56 4411.25 4443.20 4457.44
4470.50 4475.66 4612.41

Zero-point correction= 0.169620 (Hartree/Particle)
Thermal correction to Energy= 0.177463
Thermal correction to Enthalpy= 0.178407
Thermal correction to Gibbs Free Energy= 0.137518
Sum of electronic and zero-point Energies= -720.694087
Sum of electronic and thermal Energies= -720.686244
Sum of electronic and thermal Enthalpies= -720.685300
Sum of electronic and thermal Free Energies= -720.726190

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.360	31.405	86.060

ZPE(harm) = 0.44239D+03 kJ/mol ZPE(anh)= 0.43616D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.71370D-76	0.85058D-75	
QZvib	0.22720D+02	0.21956D+02	
Energy	0.46298D+03	0.45696D+03	kJ/mol
Enthalpy	0.46546D+03	0.45944D+03	kJ/mol
Entropy	0.36839D+03	0.36882D+03	J/(mol K)
Sp.Heat(V)	0.13140D+03	0.13399D+03	J/(mol K)
Sp.Heat(P)	0.13971D+03	0.14231D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.71370D-76	0.85058D-75	
QZvib	0.22720D+02	0.21956D+02	
Energy	0.46298D+03	0.45696D+03	kJ/mol
Enthalpy	0.46546D+03	0.45944D+03	kJ/mol

Entropy	0.36839D+03	0.36882D+03	J/(mol K)
Sp.Heat(V)	0.13140D+03	0.13399D+03	J/(mol K)
Sp.Heat(P)	0.13971D+03	0.14231D+03	J/(mol K)

6b-7 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -720.885422732

Zero-point correction= 0.168542 (Hartree/Particle)
Thermal correction to Energy= 0.176484
Thermal correction to Enthalpy= 0.177428
Thermal correction to Gibbs Free Energy= 0.136280
Sum of electronic and ZPE= -720.716881
Sum of electronic and thermal Energies= -720.708939
Sum of electronic and thermal Enthalpies= -720.707994
Sum of electronic and thermal Free Energies= -720.749143

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.745	31.733	86.604

C,0,2.225737,0.608357,1.249603
C,0,2.703724,-0.544357,2.111508
C,0,2.080502,-0.866605,3.330787
C,0,0.835582,-0.127224,3.836447
C,0,0.229348,0.806277,2.768513
C,0,1.2972,1.582192,1.987422
B,0,3.612623,-0.052202,3.673095
H,0,1.08713,0.434134,4.740474
H,0,3.249682,-1.331165,1.599418
H,0,1.674714,0.138491,0.421001
H,0,0.090943,-0.873536,4.125416
H,0,-0.357454,0.205317,2.059916
H,0,-0.472025,1.495727,3.251293
H,0,1.879506,2.214197,2.666383
H,0,0.825029,2.248409,1.256781
H,0,3.080349,1.126683,0.802659
H,0,4.2601,0.111646,2.63753
H,0,3.346357,1.024659,4.112553
H,0,4.254487,-0.853798,4.279033
Cl,0,2.106679,-2.60789,3.800562

B3LYP/6-31G*
E(RB3LYP) = -720.862154879

Zero-point correction= 0.169711 (Hartree/Particle)
Thermal correction to Energy= 0.177580
Thermal correction to Enthalpy= 0.178524
Thermal correction to Gibbs Free Energy= 0.137503
Sum of electronic and ZPE= -720.692444
Sum of electronic and thermal Energies= -720.684575
Sum of electronic and thermal Enthalpies= -720.683631
Sum of electronic and thermal Free Energies= -720.724652

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.433	31.401	86.336

C,0,2.2246261617,0.6049368028,1.2478903931
C,0,2.7097089696,-0.5418535097,2.1144302931
C,0,2.0857908123,-0.8639766811,3.3373909306
C,0,0.8338972619,-0.1291794418,3.8350431022
C,0,0.2323594441,0.8081032232,2.767983589
C,0,1.3027490067,1.5817299334,1.989004507
B,0,3.6030809318,-0.0539335056,3.6809101208
H,0,1.0769885129,0.4291723132,4.7435633174
H,0,3.2526513361,-1.3311549859,1.6020225401
H,0,1.6660525774,0.130731451,0.4263620157
H,0,0.0870151449,-0.8770661028,4.1159992219
H,0,-0.3553700248,0.2104509746,2.0568719747
H,0,-0.4683636161,1.4991250033,3.2505574974
H,0,1.8897801263,2.2085594756,2.6692817876
H,0,0.8333248008,2.2529741026,1.2604531221
H,0,3.0753411344,1.1212137656,0.790080242
H,0,4.2368397544,0.1210711893,2.6325560793
H,0,3.3442554473,1.0262391327,4.120140471
H,0,4.2696921059,-0.8498204027,4.2692755587
Cl,0,2.1097931123,-2.6080107375,3.8005772362

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162922	E(Thermal)=	0.171087
E(QCISD(T))=	-719.419004	E(Empiric)=	-0.155480
DE(Plus)=	-0.015382	DE(2DF)=	-0.312498
E(Delta-G3)=	-0.722237	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.461679	G3 Energy=	-720.453515
G3 Enthalpy=	-720.452571	G3 Free Energy=	-720.494098

For Anharmonic Corrections of 6b-7

Zero-point vibrational energy 445574.5 (Joules/Mol)
106.49486 (Kcal/Mol)
Warning -- explicit consideration of 11 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 153.40 274.43 357.95 435.31 445.94
(Kelvin) 511.16 575.91 626.05 667.60 784.80
851.43 1042.56 1067.41 1174.28 1194.32
1231.35 1308.06 1313.87 1379.90 1447.84
1509.01 1540.81 1572.40 1594.32 1616.23
1700.18 1718.63 1729.81 1738.99 1861.47
1882.40 1899.74 1987.27 1996.57 2009.67
2022.34 2135.24 2171.35 2187.29 2197.55
2211.19 3411.80 3736.30 3880.99 4352.85
4364.74 4408.05 4431.89 4447.62 4451.74
4471.87 4494.39 4602.18

Zero-point correction= 0.169710 (Hartree/Particle)
Thermal correction to Energy= 0.177580
Thermal correction to Enthalpy= 0.178524
Thermal correction to Gibbs Free Energy= 0.137503
Sum of electronic and zero-point Energies= -720.692445
Sum of electronic and thermal Energies= -720.684575
Sum of electronic and thermal Enthalpies= -720.683631
Sum of electronic and thermal Free Energies= -720.724652

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.433	31.401	86.336

ZPE(harm) = 0.44284D+03 kJ/mol ZPE(anh)= 0.43562D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.66594D-76	0.15629D-74	
QZvib	0.25419D+02	0.32488D+02	
Energy	0.46350D+03	0.45704D+03	kJ/mol
Enthalpy	0.46598D+03	0.45951D+03	kJ/mol
Entropy	0.36955D+03	0.37411D+03	J/(mol K)
Sp.Heat(V)	0.13138D+03	0.13562D+03	J/(mol K)
Sp.Heat(P)	0.13970D+03	0.14394D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.66594D-76	0.15629D-74	
QZvib	0.25419D+02	0.32488D+02	
Energy	0.46350D+03	0.45704D+03	kJ/mol
Enthalpy	0.46598D+03	0.45951D+03	kJ/mol
Entropy	0.36955D+03	0.37411D+03	J/(mol K)
Sp.Heat(V)	0.13138D+03	0.13562D+03	J/(mol K)
Sp.Heat(P)	0.13970D+03	0.14394D+03	J/(mol K)

6b-8 Variational Transition State

B3LYP/6-31+G**

E(RB+HF-LYP) = -720.888951220
Zero-point correction= 0.165388 (Hartree/Particle)
Thermal correction to Energy= 0.175045
Thermal correction to Enthalpy= 0.175989
Thermal correction to Gibbs Free Energy= 0.130131
Sum of electronic and zero-point Energies= -720.723563
Sum of electronic and thermal Energies= -720.713906
Sum of electronic and thermal Enthalpies= -720.712962
Sum of electronic and thermal Free Energies= -720.758821

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.842	34.809	96.517

VTS_clcyclohexeneVts_386
B3LYP/6-31G*
E(RB+HF-LYP) = -720.867829816
Zero-point correction= 0.168183 (Hartree/Particle)
Thermal correction to Energy= 0.177004
Thermal correction to Enthalpy= 0.177949
Thermal correction to Gibbs Free Energy= 0.134629
Sum of electronic and zero-point Energies= -720.699647
Sum of electronic and thermal Energies= -720.690825
Sum of electronic and thermal Enthalpies= -720.689881
Sum of electronic and thermal Free Energies= -720.733201

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.072	33.244	91.174

C,0,-0.7529,-1.38701,1.18925
C,0,0.13799,-0.16558,1.09615
C,0,0.09414,0.67406,0.03977
C,0,-0.74444,0.4486,-1.19323
C,0,-1.88991,-0.54173,-0.91202
C,0,-1.39525,-1.7776,-0.15099
B,0,2.07812,-1.0144,0.00962
H,0,-0.09689,0.08253,-2.00094
H,0,0.6808,0.13183,1.98862
H,0,-1.53597,-1.16052,1.92966
H,0,-1.14437,1.41073,-1.53026
H,0,-2.66281,-0.03205,-0.32065
H,0,-2.35774,-0.83272,-1.8596
H,0,-0.66161,-2.3125,-0.76436
H,0,-2.22542,-2.47052,0.02924
H,0,-0.18101,-2.22634,1.60049
H,0,2.23617,-1.5745,1.05626
H,0,1.5587,-1.60995,-0.88743
H,0,2.73763,-0.05105,-0.23115
Cl,0,0.94237,2.21745,0.09308

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.161455	E(Thermal)=	0.170569
E(QCISD(T))=	-719.424108	E(Empiric)=	-0.155480
DE(Plus)=	-0.015486	DE(2DF)=	-0.310941
E(Delta-G3)=	-0.722986	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.467545	G3 Energy=	-720.458432
G3 Enthalpy=	-720.457488	G3 Free Energy=	-720.501350

6b-9 Product

B3LYP/6-31+G**
E(RB3LYP) = -720.936769162

Zero-point correction= 0.171364 (Hartree/Particle)
Thermal correction to Energy= 0.179695
Thermal correction to Enthalpy= 0.180639
Thermal correction to Gibbs Free Energy= 0.138765
Sum of electronic and ZPE= -720.765405

Sum of electronic and thermal Energies= -720.757075
Sum of electronic and thermal Enthalpies= -720.756130
Sum of electronic and thermal Free Energies= -720.798004

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.760	32.772	88.130

C,0,2.103768,0.552502,1.055406
C,0,3.113136,0.211021,2.163412
C,0,2.4914,-0.332815,3.435515
C,0,1.273201,0.440785,3.903315
C,0,0.268246,0.780962,2.791086
C,0,0.95786,1.430749,1.581422
B,0,3.330426,-1.19609,4.436531
H,0,1.683467,1.375128,4.321187
H,0,3.891728,-0.467729,1.8037
H,0,1.693121,-0.380334,0.64782
H,0,0.791751,-0.080605,4.735545
H,0,-0.236995,-0.140362,2.47361
H,0,-0.508328,1.443016,3.191736
H,0,1.356228,2.413842,1.873354
H,0,0.227453,1.615031,0.784799
H,0,2.623973,1.053519,0.230625
H,0,3.630063,1.131935,2.480605
H,0,2.930625,-1.34725,5.550738
H,0,4.432687,-1.534883,4.129417
Cl,0,1.956403,-2.229106,3.12057

B3LYP/6-31G*
E(RB3LYP) = -720.914415674

Zero-point correction= 0.172530 (Hartree/Particle)
Thermal correction to Energy= 0.180812
Thermal correction to Enthalpy= 0.181756
Thermal correction to Gibbs Free Energy= 0.139977
Sum of electronic and ZPE= -720.741885
Sum of electronic and thermal Energies= -720.733604
Sum of electronic and thermal Enthalpies= -720.732660
Sum of electronic and thermal Free Energies= -720.774438

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.461	32.520	87.931

C,0,2.1046297349,0.5506799966,1.0569606921
C,0,3.1152773599,0.2163797944,2.1654638772
C,0,2.4930621954,-0.3296359981,3.4368138421
C,0,1.2759083476,0.4456868607,3.9048653497
C,0,0.2695241095,0.7794438936,2.7923330301
C,0,0.9572144536,1.4274394686,1.581073511
B,0,3.3273127129,-1.201302459,4.433931555
H,0,1.6852154223,1.3832536357,4.3174592957
H,0,3.8979007074,-0.4590218638,1.8068519111
H,0,1.6963422949,-0.3852533073,0.6533638009
H,0,0.7956507265,-0.0723052659,4.740509435
H,0,-0.2330799687,-0.1447288174,2.4779111647
H,0,-0.5092950387,1.4406775579,3.1912969221
H,0,1.3539957534,2.4120903434,1.870859171
H,0,0.225944989,1.6087677008,0.7838903946
H,0,2.622854676,1.0502109401,0.2293909922
H,0,3.6269317703,1.141190646,2.4812730379
H,0,2.9249953141,-1.3575936284,5.5476103866
H,0,4.4287718703,-1.5451045203,4.1254412582
Cl,0,1.9510555695,-2.2215589777,3.1130933727

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.165629	E(Thermal)=	0.174211
E(QCISD(T))=	-719.470339	E(Empiric)=	-0.155480
DE(Plus)=	-0.015164	DE(2DF)=	-0.313611
E(Delta-G3)=	-0.721522	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.510487	G3 Energy=	-720.501905
G3 Enthalpy=	-720.500961	G3 Free Energy=	-720.543268

6b-10 Product
B3LYP/6-31+G**
E(RB3LYP) = -720.936769113

Zero-point correction= 0.171356 (Hartree/Particle)
Thermal correction to Energy= 0.179689
Thermal correction to Enthalpy= 0.180633
Thermal correction to Gibbs Free Energy= 0.138753
Sum of electronic and ZPE= -720.765413
Sum of electronic and thermal Energies= -720.757080
Sum of electronic and thermal Enthalpies= -720.756136

Sum of electronic and thermal Free Energies= -720.798016

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.756	32.776	88.143

C,0,2.0652337978,0.5502229894,1.0362199851
C,0,3.0403312596,0.1602369692,2.158729674
C,0,2.3742178664,-0.3582274396,3.4189275233
C,0,1.184820078,0.4679393545,3.8697883252
C,0,0.2145393193,0.857452124,2.743055955
C,0,0.9524020368,1.4786504023,1.5468537985
B,0,3.1556131072,-1.2631511864,4.429692236
H,0,1.630211775,1.3810641117,4.2986211204
H,0,3.7929476856,-0.5522329869,1.8090327991
H,0,1.6188251956,-0.3620049332,0.6196681007
H,0,0.6666612873,-0.0340308559,4.6918778505
H,0,-0.3273676894,-0.0386917619,2.414070473
H,0,-0.537066189,1.5531899899,3.1340779665
H,0,1.3905095667,2.4416826986,1.8484978802
H,0,0.2440708841,1.6982954636,0.7393456431
H,0,2.6207338979,1.0286269129,0.2211042558
H,0,3.5934655404,1.0556663803,2.4877203578
H,0,2.7313209836,-1.398823991,5.5368282026
H,0,4.2466923658,-1.6507777996,4.140724362
Cl,0,1.7592232313,-2.2294744421,3.0880524912

B3LYP/6-31G*
E(RB3LYP) = -720.914415819

Zero-point correction= 0.172533 (Hartree/Particle)
Thermal correction to Energy= 0.180814
Thermal correction to Enthalpy= 0.181758
Thermal correction to Gibbs Free Energy= 0.139980
Sum of electronic and ZPE= -720.741883
Sum of electronic and thermal Energies= -720.733602
Sum of electronic and thermal Enthalpies= -720.732657
Sum of electronic and thermal Free Energies= -720.774436

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.463	32.521	87.931

C,0,2.0653090069,0.5466024814,1.037144878
C,0,3.0420558466,0.1628175478,2.1601346272
C,0,2.3753682563,-0.3557779412,3.4202733566
C,0,1.1893320682,0.4752929998,3.8722093719
C,0,0.2169073972,0.8586624676,2.7454134975
C,0,0.9528516176,1.4755356324,1.5463785079
B,0,3.1509789317,-1.2698809842,4.4267371016
H,0,1.6364932877,1.3914194119,4.2935253727
H,0,3.7975018575,-0.547939737,1.8117695595
H,0,1.6196695567,-0.3682596706,0.624923646
H,0,0.6724317453,-0.021213856,4.6989138827
H,0,-0.3241325738,-0.0400172074,2.4211888784
H,0,-0.5355344925,1.555385876,3.1344423677
H,0,1.3913507712,2.4397214789,1.84468773
H,0,0.2430390396,1.692804713,0.7388920004
H,0,2.6191507927,1.022809849,0.2189926954
H,0,3.5914025975,1.0620231174,2.4864502189
H,0,2.7247597896,-1.409440135,5.5336742033
H,0,4.2393722407,-1.6651783191,4.1341114779
Cl,0,1.7490782632,-2.2197557249,3.0830256262

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.165636	E(Thermal)=	0.174217
E(QCISD(T))=	-719.470341	E(Empiric)=	-0.155480
DE(Plus)=	-0.015162	DE(2DF)=	-0.313615
E(Delta-G3)=	-0.721522	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.510485	G3 Energy=	-720.501904
G3 Enthalpy=	-720.500960	G3 Free Energy=	-720.543266

6b-11 Product
B3LYP/6-31+G**
E(RB3LYP) = -720.936026531

Zero-point correction= 0.171611 (Hartree/Particle)
Thermal correction to Energy= 0.179968
Thermal correction to Enthalpy= 0.180912
Thermal correction to Gibbs Free Energy= 0.138929
Sum of electronic and ZPE= -720.764416
Sum of electronic and thermal Energies= -720.756059
Sum of electronic and thermal Enthalpies= -720.755115
Sum of electronic and thermal Free Energies= -720.797098

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.932	32.727	88.361

C,0,1.9497504285,0.6179373006,0.9798419684
C,0,2.890075149,-0.006570038,2.0370856764
C,0,2.038244701,-0.5868339613,3.1516139274
C,0,1.1866461177,0.4630837669,3.8420934806
C,0,0.2392483839,1.0894116644,2.7922647537
C,0,1.0204925995,1.6701752907,1.603777997
Cl,0,3.1920454644,-1.4567035657,4.4661503241
H,0,1.8232070874,1.2509420468,4.2667669199
H,0,3.5143573919,-0.7826016038,1.5852068876
H,0,1.3485295441,-0.1759535582,0.5159858484
H,0,0.6129920921,0.0174714289,4.659720027
H,0,-0.4611140203,0.3227927042,2.4335480948
H,0,-0.3657797272,1.8656801735,3.274838989
H,0,1.6198895718,2.5254755438,1.9470204801
H,0,0.3263509673,2.0567884168,0.848078878
H,0,2.5549494248,1.0606969052,0.1803282009
H,0,3.5546107444,0.7735055735,2.4322540768
B,0,1.5765748162,-2.0850279606,3.1057425426
H,0,0.6633581522,-2.437245836,3.7883147478
H,0,2.0630481113,-2.8233012915,2.3044701796

B3LYP/6-31G*
E(RB3LYP) = -720.913703767

Zero-point correction= 0.172782 (Hartree/Particle)
Thermal correction to Energy= 0.181096
Thermal correction to Enthalpy= 0.182040
Thermal correction to Gibbs Free Energy= 0.140129
Sum of electronic and ZPE= -720.740921
Sum of electronic and thermal Energies= -720.732608
Sum of electronic and thermal Enthalpies= -720.731664
Sum of electronic and thermal Free Energies= -720.773575

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.639	32.475	88.209

C,0,1.960691791,0.6247110422,0.9988716636
C,0,2.8526464827,-0.0236284763,2.0828741809
C,0,1.9510064971,-0.5997935807,3.1589551676

C,0,1.0941601434,0.4579626297,3.8295550108
C,0,0.195324103,1.1086554389,2.7526745066
C,0,1.0287440401,1.6873446057,1.599731867
Cl,0,3.0416941834,-1.5037490344,4.5066174878
H,0,1.7278310366,1.2321530042,4.2834151224
H,0,3.4813321123,-0.8051312958,1.6458707049
H,0,1.3622162257,-0.155850078,0.5088409442
H,0,0.4840832044,0.0157000186,4.6227726053
H,0,-0.5026409718,0.355584692,2.3611235673
H,0,-0.4155309924,1.8901137127,3.2202832928
H,0,1.6309993953,2.5279001489,1.973972973
H,0,0.3693516295,2.0949041177,0.8235761389
H,0,2.6003878566,1.0632013019,0.2236279174
H,0,3.5144532639,0.7430702498,2.50836855
B,0,1.4702625186,-2.0900338568,3.086001249
H,0,0.5266366782,-2.4333436254,3.7326073298
H,0,1.9738278025,-2.8300480152,2.2953637206

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.165871	E(Thermal)=	0.174482
E(QCISD(T))=	-719.470446	E(Empiric)=	-0.155480
DE(Plus)=	-0.014931	DE(2DF)=	-0.313423
E(Delta-G3)=	-0.721676	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.510085	G3 Energy=	-720.501474
G3 Enthalpy=	-720.500530	G3 Free Energy=	-720.542968

6b-12 Product
B3LYP/6-31+G**
E(RB3LYP) = -720.928967549

Zero-point correction= 0.170564 (Hartree/Particle)
Thermal correction to Energy= 0.179079
Thermal correction to Enthalpy= 0.180023
Thermal correction to Gibbs Free Energy= 0.137529
Sum of electronic and ZPE= -720.758403
Sum of electronic and thermal Energies= -720.749889
Sum of electronic and thermal Enthalpies= -720.748945
Sum of electronic and thermal Free Energies= -720.791438

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.374	32.891	89.436

C,0,2.0835777028,0.5481441802,1.0596793993
C,0,3.029973581,0.07428723,2.1641958682
C,0,2.3069602548,-0.493248494,3.3959825596
C,0,1.1619938112,0.4227737066,3.8822117973
C,0,0.2071887726,0.8214040043,2.7457929242
C,0,0.9647971714,1.4649821295,1.5741062455
B,0,3.260238445,-1.0711553881,4.4966407621
H,0,1.5944556319,1.3282384548,4.3266177709
H,0,3.7458778257,-0.6519215322,1.7744006663
H,0,1.6381002177,-0.3607414812,0.6266806355
H,0,0.6129661268,-0.0843423397,4.6838607603
H,0,-0.3234217615,-0.0738693267,2.387693004
H,0,-0.5599576035,1.5091561312,3.1218048875
H,0,1.3989828491,2.4193395106,1.8974134504
H,0,0.2760226128,1.6946445531,0.7525288206
H,0,2.6550996158,1.0319201759,0.2607820435
Cl,0,4.1169814739,1.4827890467,2.7013357795
H,0,2.8981123779,-1.1574828806,5.6334788656
H,0,4.3251029575,-1.5218009232,4.1921698635
H,0,1.8397969372,-1.439711757,3.0346488959

B3LYP/6-31G*
E(RB3LYP) = -720.905953820

Zero-point correction= 0.171692 (Hartree/Particle)
Thermal correction to Energy= 0.180197
Thermal correction to Enthalpy= 0.181141
Thermal correction to Gibbs Free Energy= 0.138592
Sum of electronic and ZPE= -720.734262
Sum of electronic and thermal Energies= -720.725757
Sum of electronic and thermal Enthalpies= -720.724813
Sum of electronic and thermal Free Energies= -720.767362

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.075	32.655	89.552

C,0,2.0840263088,0.54960475,1.0603571651
C,0,3.0272519355,0.0702637168,2.1650900059
C,0,2.3001729345,-0.5032200491,3.3922681302
C,0,1.157699004,0.4148126626,3.8797068611
C,0,0.2059183524,0.8182434353,2.7431371741
C,0,0.9671261947,1.4667049732,1.5771617559

B,0,3.2655107569,-1.0611283906,4.4958603435
H,0,1.5919886546,1.3181332078,4.327210363
H,0,3.7436444135,-0.6551661142,1.7738388705
H,0,1.6370734576,-0.356884383,0.6229986691
H,0,0.6060675769,-0.0927701798,4.6800476567
H,0,-0.3240341368,-0.0754514457,2.3792459803
H,0,-0.5628230167,1.5044328224,3.1201777373
H,0,1.4041817627,2.4177446785,1.9072612297
H,0,0.2805627829,1.7035605799,0.755153703
H,0,2.6582273646,1.0352200368,0.2639075605
Cl,0,4.1107659483,1.4754919733,2.7144657353
H,0,2.9241086555,-1.1120339999,5.6422466165
H,0,4.3232023574,-1.5282964906,4.1868992162
H,0,1.8321776926,-1.4458567837,3.0249902262

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.164824	E(Thermal)=	0.173623
E(QCISD(T))=	-719.463234	E(Empiric)=	-0.155480
DE(Plus)=	-0.015026	DE(2DF)=	-0.311883
E(Delta-G3)=	-0.722449	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.503247	G3 Energy=	-720.494448
G3 Enthalpy=	-720.493504	G3 Free Energy=	-720.536584

6b-13 Product
B3LYP/6-31+G**
E(RB3LYP) = -720.929949507

Zero-point correction= 0.171145 (Hartree/Particle)
Thermal correction to Energy= 0.179739
Thermal correction to Enthalpy= 0.180683
Thermal correction to Gibbs Free Energy= 0.138014
Sum of electronic and ZPE= -720.758804
Sum of electronic and thermal Energies= -720.750211
Sum of electronic and thermal Enthalpies= -720.749267
Sum of electronic and thermal Free Energies= -720.791935

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.788	32.890	89.804

C,0,2.043673,0.477185,1.014631
C,0,2.992881,0.005953,2.112967

C,0,2.277206,-0.63383,3.305607
C,0,1.232164,0.381592,3.879803
C,0,0.265832,0.874709,2.788666
C,0,1.020276,1.472384,1.592913
B,0,3.206241,-1.030393,4.506035
H,0,1.752572,1.247327,4.314607
Cl,0,4.200113,-1.202281,1.414093
H,0,1.521495,-0.392957,0.596741
H,0,0.670953,-0.090157,4.694853
H,0,-0.349431,0.030795,2.447468
H,0,-0.421033,1.61714,3.213217
H,0,1.539295,2.388457,1.909462
H,0,0.316309,1.770479,0.807141
H,0,2.611454,0.935703,0.19822
H,0,3.621644,0.834613,2.453777
H,0,2.859966,-1.86816,5.286202
H,0,4.220897,-0.431232,4.714128
H,0,1.710231,-1.503913,2.943375

B3LYP/6-31G*
E(RB3LYP) = -720.907077049

Zero-point correction= 0.172280 (Hartree/Particle)
Thermal correction to Energy= 0.180845
Thermal correction to Enthalpy= 0.181790
Thermal correction to Gibbs Free Energy= 0.139153
Sum of electronic and ZPE= -720.734797
Sum of electronic and thermal Energies= -720.726232
Sum of electronic and thermal Enthalpies= -720.725288
Sum of electronic and thermal Free Energies= -720.767924

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.482	32.662	89.736

C,0,2.0434897632,0.475166232,1.01507252
C,0,2.9919173655,0.0056756945,2.1148721396
C,0,2.2733069295,-0.6338152055,3.306216583
C,0,1.2328458348,0.3854226149,3.8801014976
C,0,0.2664314063,0.875682704,2.7885845402
C,0,1.0209290503,1.4713748629,1.5922044024
B,0,3.2067290805,-1.0333352195,4.502845705
H,0,1.7574075361,1.2510676934,4.310610175
Cl,0,4.1999687192,-1.2028655117,1.4214152676

H,0,1.5211307683,-0.3958595875,0.598589115
H,0,0.6720364264,-0.0812145867,4.6990460706
H,0,-0.3484609539,0.0305177849,2.448764258
H,0,-0.4218281603,1.618616087,3.2111375403
H,0,1.5414168478,2.3871338864,1.9083564482
H,0,0.3167070344,1.7701380973,0.8063082128
H,0,2.611509466,0.9321727274,0.1973868644
H,0,3.6170135425,0.8363272033,2.4576938113
H,0,2.8788535019,-1.8928816968,5.2685273461
H,0,4.2081997743,-0.4155045432,4.7253756523
H,0,1.7031340672,-1.5004052369,2.9407978508

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.165389	E(Thermal)=	0.174245
E(QCISD(T))=	-719.464356	E(Empiric)=	-0.155480
DE(Plus)=	-0.014825	DE(2DF)=	-0.311313
E(Delta-G3)=	-0.722266	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.502852	G3 Energy=	-720.493996
G3 Enthalpy=	-720.493051	G3 Free Energy=	-720.536218

6b-14 Product
B3LYP/6-31+G**
E(RB3LYP) = -720.928656754

Zero-point correction= 0.170683 (Hartree/Particle)
Thermal correction to Energy= 0.179109
Thermal correction to Enthalpy= 0.180053
Thermal correction to Gibbs Free Energy= 0.137822
Sum of electronic and ZPE= -720.757974
Sum of electronic and thermal Energies= -720.749548
Sum of electronic and thermal Enthalpies= -720.748604
Sum of electronic and thermal Free Energies= -720.790834

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.392	32.796	88.882

C,0,2.0425426644,0.545145196,1.0238894994
C,0,2.9844919996,-0.0163190434,2.0934588896
C,0,2.2112729209,-0.5969768606,3. 281760452
C,0,1.1974337413,0.4100217291,3.8675438662

C,0,0.2353452575,0.9087730966,2.7761204106
C,0,0.9992506261,1.5200136484,1.5906838976
H,0,2.9487855476,-0.8570357229,4.0754200453
H,0,1.7304157738,1.2667453547,4.2979186103
H,0,3.6533637077,-0.7624129093,1.6622286977
H,0,1.5293914515,-0.3220214906,0.5792657177
H,0,0.6378099842,-0.0637099873,4.6816580352
H,0,-0.3778490015,0.0659170291,2.4207317551
H,0,-0.4611778345,1.6450327583,3.1945422874
H,0,1.5054318252,2.4372776567,1.9161840009
H,0,0.3024200651,1.810251238,0.7955237097
H,0,2.6232200421,1.01325255,0.2228088165
Cl,0,4.1566340572,1.3156945501,2.6489080506
B,0,1.6863474826,-2.0500612176,3.0431529985
H,0,0.8255396106,-2.49363194,3.7452646515
H,0,2.1980160787,-2.7699086354,2.2349836083

B3LYP/6-31G*
E(RB3LYP) = -720.905645958

Zero-point correction= 0.171816 (Hartree/Particle)
Thermal correction to Energy= 0.180210
Thermal correction to Enthalpy= 0.181155
Thermal correction to Gibbs Free Energy= 0.138969
Sum of electronic and ZPE= -720.733830
Sum of electronic and thermal Energies= -720.725436
Sum of electronic and thermal Enthalpies= -720.724491
Sum of electronic and thermal Free Energies= -720.766677

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.084	32.551	88.786

C,0,2.0434619513,0.5408501047,1.0256323043
C,0,2.9876711236,-0.0136868868,2.0968237867
C,0,2.2157449536,-0.5958345448,3.2857234099
C,0,1.2006325733,0.4110385753,3.8691820464
C,0,0.2378303451,0.9056562098,2.7774318472
C,0,1.0000597484,1.5155686526,1.5908804605
H,0,2.9536302397,-0.8510496968,4.0795561912
H,0,1.7333450255,1.2690678621,4.2979469141
H,0,3.6587862451,-0.7590238479,1.6667838038
H,0,1.5309372214,-0.3292696353,0.5847980542
H,0,0.6412811482,-0.0617354266,4.6847257933

H,0,-0.3735813044,0.0601827079,2.4236803431
H,0,-0.460985348,1.6412143059,3.1944983222
H,0,1.5065427437,2.433581824,1.9146848609
H,0,0.3021240416,1.804404896,0.7954952282
H,0,2.6222443362,1.0072595547,0.2216474752
Cl,0,4.149785617,1.3246614524,2.6511574008
B,0,1.6797685872,-2.0448223963,3.0359853625
H,0,0.8178895324,-2.489913147,3.7376342711
H,0,2.1815172191,-2.7621035638,2.2177801243

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.164943	E(Thermal)=	0.173634
E(QCISD(T))=	-719.462867	E(Empiric)=	-0.155480
DE(Plus)=	-0.014612	DE(2DF)=	-0.311986
E(Delta-G3)=	-0.722832	E(G3-Empiric)=	-0.155480
G3(0 K)=	-720.502834	G3 Energy=	-720.494143
G3 Enthalpy=	-720.493199	G3 Free Energy=	-720.535913

6c-1 Starting Material
B3LYP/6-31+G**
E(RB3LYP) = -193.133106302

Zero-point correction= 0.085224 (Hartree/Particle)
Thermal correction to Energy= 0.089980
Thermal correction to Enthalpy= 0.090924
Thermal correction to Gibbs Free Energy= 0.058502
Sum of electronic and ZPE= -193.047883
Sum of electronic and thermal Energies= -193.043126
Sum of electronic and thermal Enthalpies= -193.042182
Sum of electronic and thermal Free Energies= -193.074604

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	56.463	15.884	68.237

C,0,2.6020522114,-0.2556549802,1.8408524052
C,0,1.8788413566,-0.7104602255,2.873170569
O,0,0.6444960494,-0.3081324832,3.2738356397
C,0,0.0210546081,0.7241435711,2.5179325189
H,0,2.2693505631,0.5271213394,1.1699924363
H,0,3.5778000288,-0.6891281456,1.6574457609
H,0,2.2390682923,-1.4971910103,3.5293619051
H,0,-0.9462160242,0.9032733479,2.9883970164

H,0,0.6205011237,1.642928946,2.5411494677
H,0,-0.1253772091,0.4125116403,1.4760702809

B3LYP/6-31G*
E(RB3LYP) = -193.114063710

Zero-point correction= 0.085796 (Hartree/Particle)
Thermal correction to Energy= 0.090526
Thermal correction to Enthalpy= 0.091470
Thermal correction to Gibbs Free Energy= 0.059100
Sum of electronic and ZPE= -193.028267
Sum of electronic and thermal Energies= -193.023537
Sum of electronic and thermal Enthalpies= -193.022593
Sum of electronic and thermal Free Energies= -193.054963

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	56.806	15.760	68.129

C,0,2.5989473262,-0.2549435432,1.8421205134
C,0,1.8758985441,-0.7071781226,2.8715196182
O,0,0.642777713,-0.3093663346,3.277285155
C,0,0.0248240279,0.7200544975,2.5199819466
H,0,2.2668598625,0.5285146005,1.1710130905
H,0,3.5753112981,-0.6873071017,1.6564487762
H,0,2.2370220917,-1.4947525771,3.5276041859
H,0,-0.9447319618,0.9039287409,2.9862887106
H,0,0.6245622662,1.6396937687,2.5396148661
H,0,-0.1199001678,0.4107680715,1.4763311375

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.082365	E(Thermal)=	0.087210
E(QCISD(T))=	-192.533386	E(Empiric)=	-0.081120
DE(Plus)=	-0.014377	DE(2DF)=	-0.168129
E(Delta-G3)=	-0.244745	E(G3-Empiric)=	-0.081120
G3(0 K)=	-192.959391	G3 Energy=	-192.954546
G3 Enthalpy=	-192.953602	G3 Free Energy=	-192.986167

For Anharmonic Corrections of 6c-1

Zero-point vibrational energy 225258.6 (Joules/Mol)
53.83810 (Kcal/Mol)
Warning -- explicit consideration of 4 degrees of freedom as
vibrations may cause significant error

Vibrational temperatures: 346.49 373.34 464.36 859.19 1036.91
(Kelvin) 1183.87 1322.89 1437.26 1499.82 1711.30
1770.40 1813.52 1972.33 2087.15 2167.96
2182.73 2211.29 2469.41 4357.29 4440.95
4546.24 4596.42 4618.20 4715.39

Zero-point correction= 0.085796 (Hartree/Particle)
Thermal correction to Energy= 0.090526
Thermal correction to Enthalpy= 0.091471
Thermal correction to Gibbs Free Energy= 0.059100
Sum of electronic and zero-point Energies= -193.028267
Sum of electronic and thermal Energies= -193.023537
Sum of electronic and thermal Enthalpies= -193.022593
Sum of electronic and thermal Free Energies= -193.054963

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.806	15.760	68.129

ZPE(harm) = 0.22526D+03 kJ/mol ZPE(anh)= 0.22178D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.10287D-38	0.48295D-38	
QZvib	0.29912D+01	0.34454D+01	
Energy	0.23768D+03	0.23450D+03	kJ/mol
Enthalpy	0.24016D+03	0.23698D+03	kJ/mol
Entropy	0.28505D+03	0.28726D+03	J/(mol K)
Sp.Heat(V)	0.65940D+02	0.67300D+02	J/(mol K)
Sp.Heat(P)	0.74254D+02	0.75614D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.10287D-38	0.48295D-38	
QZvib	0.29912D+01	0.34454D+01	
Energy	0.23768D+03	0.23450D+03	kJ/mol
Enthalpy	0.24016D+03	0.23698D+03	kJ/mol
Entropy	0.28505D+03	0.28726D+03	J/(mol K)
Sp.Heat(V)	0.65940D+02	0.67300D+02	J/(mol K)
Sp.Heat(P)	0.74254D+02	0.75614D+02	J/(mol K)

6c-2 Starting Material

B3LYP/6-31+G**
E(RB3LYP) = -193.129940063

Zero-point correction= 0.084180 (Hartree/Particle)
Thermal correction to Energy= 0.089503
Thermal correction to Enthalpy= 0.090447
Thermal correction to Gibbs Free Energy= 0.055806
Sum of electronic and zero-point Energies= -193.045760
Sum of electronic and thermal Energies= -193.040437
Sum of electronic and thermal Enthalpies= -193.039493
Sum of electronic and thermal Free Energies= -193.074134

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.164	16.402	72.909

H,0,2.1424906304,0.5979866485,1.2907583764
C,0,2.4554395159,-0.2873613624,1.833607958
C,0,1.8600851821,-0.6566633467,2.9706743335
O,0,0.8178897744,0.0374202033,3.510437215
H,0,3.2664062811,-0.8840821233,1.4346552349
H,0,2.1665864908,-1.5439050626,3.5256888631
C,0,0.3874736996,-0.3974634771,4.7967072242
H,0,-0.4768974987,0.214724705,5.057585214
H,0,0.0893928106,-1.454030632,4.7787678321
H,0,1.1743431139,-0.2520935528,5.5481147488

B3LYP/6-31+G**
E(RB3LYP) = -193.110424990

Zero-point correction= 0.084750 (Hartree/Particle)
Thermal correction to Energy= 0.090016
Thermal correction to Enthalpy= 0.090960
Thermal correction to Gibbs Free Energy= 0.056765
Sum of electronic and zero-point Energies= -193.025675
Sum of electronic and thermal Energies= -193.020409
Sum of electronic and thermal Enthalpies= -193.019465
Sum of electronic and thermal Free Energies= -193.053660

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.486	16.284	71.971

H,0,2.1840414904,0.6308852123,1.3309632407
C,0,2.4630127334,-0.281739231,1.8472147981
C,0,1.8356220594,-0.6747341703,2.9555641702

O,0,0.7926914793,0.0188657517,3.4931637303
H,0,3.2640599344,-0.8846113614,1.436274128
H,0,2.1085382176,-1.5894907833,3.484597428
C,0,0.3977497541,-0.3894782229,4.7944560665
H,0,-0.4938622815,0.1885482876,5.0456370355
H,0,0.1504230264,-1.4601529082,4.822206351
H,0,1.1809335865,-0.1835605744,5.5369200516

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.081360	E(Thermal)=	0.086730
E(QCISD(T))=	-192.529417	E(Empiric)=	-0.081120
DE(Plus)=	-0.014836	DE(2DF)=	-0.167832
E(Delta-G3)=	-0.244656	E(G3-Empiric)=	-0.081120
G3(0 K)=	-192.956500	G3 Energy=	-192.951131
G3 Enthalpy=	-192.950186	G3 Free Energy=	-192.984588

For Anharmonic Corrections of 6c-2

Zero-point vibrational energy 222512.2 (Joules/Mol)
53.18170 (Kcal/Mol)
Warning -- explicit consideration of 4 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 67.68 242.86 454.94 756.72 1019.50
(Kelvin) 1199.77 1284.36 1415.00 1611.17 1691.12
1706.66 1834.76 1955.99 2083.08 2169.03
2188.16 2204.77 2501.69 4342.64 4424.00
4521.06 4539.44 4592.18 4717.50

Zero-point correction= 0.084750 (Hartree/Particle)
Thermal correction to Energy= 0.090016
Thermal correction to Enthalpy= 0.090961
Thermal correction to Gibbs Free Energy= 0.056765
Sum of electronic and zero-point Energies= -193.025675
Sum of electronic and thermal Energies= -193.020409
Sum of electronic and thermal Enthalpies= -193.019464
Sum of electronic and thermal Free Energies= -193.053660

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	56.486	16.284	71.970

ZPE(harm) = 0.22251D+03 kJ/mol ZPE(anh)= 0.21862D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00
Harmonic value SPT anharmonic value

Qvib	0.13992D-37	0.15652D-37	
QZvib	0.13437D+02	0.31287D+01	
Energy	0.23634D+03	0.23048D+03	kJ/mol
Enthalpy	0.23882D+03	0.23296D+03	kJ/mol
Entropy	0.30112D+03	0.29073D+03	J/(mol K)
Sp.Heat(V)	0.68134D+02	0.61140D+02	J/(mol K)
Sp.Heat(P)	0.76448D+02	0.69454D+02	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.13992D-37	0.15652D-37	
QZvib	0.13437D+02	0.31287D+01	
Energy	0.23634D+03	0.23048D+03	kJ/mol
Enthalpy	0.23882D+03	0.23296D+03	kJ/mol
Entropy	0.30112D+03	0.29073D+03	J/(mol K)
Sp.Heat(V)	0.68134D+02	0.61140D+02	J/(mol K)
Sp.Heat(P)	0.76448D+02	0.69454D+02	J/(mol K)

6c-3 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -219.761728852

Zero-point correction= 0.116772 (Hartree/Particle)
Thermal correction to Energy= 0.122883
Thermal correction to Enthalpy= 0.123827
Thermal correction to Gibbs Free Energy= 0.087856
Sum of electronic and ZPE= -219.644956
Sum of electronic and thermal Energies= -219.638846
Sum of electronic and thermal Enthalpies= -219.637902
Sum of electronic and thermal Free Energies= -219.673873

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	77.110	21.814	75.707

O,0,2.31305517,0.5564536981,1.2620413146
C,0,2.5829068569,-0.4674812132,2.1028635921
C,0,1.8494186985,-0.8362564033,3.2678454156
H,0,0.9665168051,-0.2625977399,3.5255343876
C,0,1.3911428911,1.5717396741,1.6811610948
B,0,3.2889732652,-0.1650655245,3.8715373985
H,0,3.1898087413,-1.2113403396,1.5969272443

H,0,3.9412958833,0.1531738005,2.8472511697
H,0,3.0594031302,0.8804786556,4.4119353228
H,0,3.9849581879,-1.0067097732,4.3667222564
H,0,1.763055921,-1.9004067357,3.459979393
H,0,1.3756984185,2.2988588196,0.8694473563
H,0,0.3878336153,1.1561945846,1.8213208912
H,0,1.7349214157,2.050588497,2.6022181631

B3LYP/6-31G*
E(RB3LYP) = -219.741081788

Zero-point correction= 0.117609 (Hartree/Particle)
Thermal correction to Energy= 0.123658
Thermal correction to Enthalpy= 0.124602
Thermal correction to Gibbs Free Energy= 0.088733
Sum of electronic and ZPE= -219.623473
Sum of electronic and thermal Energies= -219.617424
Sum of electronic and thermal Enthalpies= -219.616480
Sum of electronic and thermal Free Energies= -219.652348

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	77.596	21.525	75.492

O,0,2.3114238258,0.5511038382,1.2561808128
C,0,2.5908862012,-0.4608140385,2.1072987907
C,0,1.8529433812,-0.8388995407,3.2741966969
H,0,0.9585748848,-0.2744362561,3.5166511481
C,0,1.4017900837,1.5688845512,1.6828225614
B,0,3.2715101425,-0.1656443839,3.8820634188
H,0,3.1930667955,-1.2095946696,1.6008971287
H,0,3.9105386811,0.1573925687,2.837430697
H,0,3.0531349205,0.8851856037,4.4174991062
H,0,3.9949408937,-0.9959470547,4.3572681436
H,0,1.7590852527,-1.9067249213,3.4468114508
H,0,1.3687496812,2.2892387012,0.8644690208
H,0,0.3993167149,1.1596866071,1.8506924855
H,0,1.7630275411,2.0581989947,2.5925035386

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.112904	E(Thermal)=	0.119129
E(QCISD(T))=	-219.032600	E(Empiric)=	-0.101400
DE(Plus)=	-0.014195	DE(2DF)=	-0.210595
E(Delta-G3)=	-0.292933	E(G3-Empiric)=	-0.101400

G3(0 K)= -219.538819 G3 Energy= -219.532594
G3 Enthalpy= -219.531650 G3 Free Energy= -219.567829

For Anharmonic Corrections of 6c-3

Zero-point vibrational energy 308783.1 (Joules/Mol)
73.80094 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 180.02 258.41 359.09 478.87 640.31
(Kelvin) 797.56 1032.92 1073.11 1130.63 1290.45
1344.55 1474.43 1494.27 1545.30 1660.57
1691.46 1700.90 1746.45 1779.78 1817.42
1915.28 2070.03 2164.71 2191.47 2204.10
2214.06 3214.80 3676.70 3816.11 4398.84
4506.82 4557.48 4567.33 4617.02 4664.84

Zero-point correction= 0.117609 (Hartree/Particle)
Thermal correction to Energy= 0.123658
Thermal correction to Enthalpy= 0.124603
Thermal correction to Gibbs Free Energy= 0.088734
Sum of electronic and zero-point Energies= -219.623473
Sum of electronic and thermal Energies= -219.617423
Sum of electronic and thermal Enthalpies= -219.616479
Sum of electronic and thermal Free Energies= -219.652347

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.597	21.524	75.491

ZPE(harm) = 0.30878D+03 kJ/mol ZPE(anh)= 0.30440D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.76922D-53	0.50591D-52	
QZvib	0.96040D+01	0.10787D+02	
Energy	0.32467D+03	0.32062D+03	kJ/mol
Enthalpy	0.32714D+03	0.32310D+03	kJ/mol
Entropy	0.32417D+03	0.32628D+03	J/(mol K)
Sp.Heat(V)	0.90058D+02	0.91855D+02	J/(mol K)
Sp.Heat(P)	0.98373D+02	0.10017D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.76922D-53	0.50591D-52	
QZvib	0.96040D+01	0.10787D+02	
Energy	0.32467D+03	0.32062D+03	kJ/mol
Enthalpy	0.32714D+03	0.32310D+03	kJ/mol
Entropy	0.32417D+03	0.32628D+03	J/(mol K)
Sp.Heat(V)	0.90058D+02	0.91855D+02	J/(mol K)
Sp.Heat(P)	0.98373D+02	0.10017D+03	J/(mol K)

6c-4 Transition State

G** E(RB3LYP) = -219.755248890

Zero-point correction= 0.116408 (Hartree/Particle)
Thermal correction to Energy= 0.122477
Thermal correction to Enthalpy= 0.123421
Thermal correction to Gibbs Free Energy= 0.087654
Sum of electronic and zero-point Energies= -219.639081
Sum of electronic and thermal Energies= -219.633012
Sum of electronic and thermal Enthalpies= -219.632068
Sum of electronic and thermal Free Energies= -219.667834

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	76.855	21.970	75.277

H,0,2.0338236622,0.6152464163,1.3348425854
C,0,2.490655508,-0.2229231718,1.8467324861
C,0,1.9098573035,-0.7230205993,2.9971422133
O,0,0.6344866841,-0.2965896526,3.3086535591
B,0,3.2437629363,0.2328980668,3.4975018967
H,0,3.2925649422,-0.7537544595,1.3516007306
H,0,3.6353311272,1.1923052051,2.8594019382
H,0,2.6175514736,0.758208534,4.378419181
H,0,4.1389456017,-0.5067480516,3.7949330723
H,0,2.1586760156,-1.7196299054,3.3601354186
C,0,0.2275809047,-0.5416626887,4.6512101251
H,0,-0.8215300202,-0.2494354703,4.7125821061
H,0,0.3251322396,-1.6063504065,4.9042476356
H,0,0.8210126216,0.0541891834,5.355310052

G* E(RB3LYP) = -219.734794645

Zero-point correction= 0.117084 (Hartree/Particle)
Thermal correction to Energy= 0.123570
Thermal correction to Enthalpy= 0.124515
Thermal correction to Gibbs Free Energy= 0.087651
Sum of electronic and zero-point Energies= -219.627099
Sum of electronic and thermal Energies= -219.620613
Sum of electronic and thermal Enthalpies= -219.619669
Sum of electronic and thermal Free Energies= -219.656532

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.542	22.690	77.585

H,0,2.0354667997,0.596350974,1.3218226001
C,0,2.488312238,-0.2396971727,1.8410100642
C,0,1.9100512043,-0.7179489248,2.9999412782
O,0,0.6403583281,-0.2853309727,3.3043293072
B,0,3.2532644712,0.2348223833,3.4810297838
H,0,3.2898583229,-0.7767429649,1.3517042168
H,0,3.5820815477,1.261080794,2.9220888903
H,0,2.6236441389,0.6480105138,4.4215091831
H,0,4.1716872064,-0.4948431891,3.7311532755
H,0,2.1660935298,-1.7046897536,3.3861358832
C,0,0.2281265654,-0.5281565575,4.6414906219
H,0,-0.819894058,-0.2286293165,4.700212958
H,0,0.3170602329,-1.5934856585,4.8986846577
H,0,0.8217404727,0.0619928453,5.35160028

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.112401	E(Thermal)=	0.119067
E(QCISD(T))=	-219.034548	E(Empiric)=	-0.101400
DE(Plus)=	-0.014570	DE(2DF)=	-0.209949
E(Delta-G3)=	-0.293049	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.541116	G3 Energy=	-219.534450
G3 Enthalpy=	-219.533506	G3 Free Energy=	-219.570701

6c-5 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -219.741081782

Zero-point correction= 0.117609 (Hartree/Particle)
Thermal correction to Energy= 0.123658
Thermal correction to Enthalpy= 0.124602

Thermal correction to Gibbs Free Energy= 0.088733
Sum of electronic and zero-point Energies= -219.623473
Sum of electronic and thermal Energies= -219.617424
Sum of electronic and thermal Enthalpies= -219.616480
Sum of electronic and thermal Free Energies= -219.652348

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.596	21.525	75.492

O,0,2.3452919475,0.5679639984,1.2737086352
C,0,2.703094656,-0.3996529074,2.1467310801
C,0,2.0426864137,-0.7515020652,3.3670663394
H,0,1.1454559681,-0.2043454596,3.6370507735
C,0,1.4284973417,1.574925012,1.7105745811
B,0,3.4703144111,-0.0122924773,3.8676368453
H,0,3.3001350265,-1.1503064102,1.6370249283
H,0,4.040463003,0.2866551313,2.7769823403
H,0,3.248302261,1.0525740861,4.3730099086
H,0,4.2447948387,-0.8007352435,4.3335994843
H,0,1.9924845914,-1.8137033604,3.586290379
H,0,1.3276948961,2.2599855465,0.8678201124
H,0,0.4502782429,1.1434126227,1.9502840691
H,0,1.8233394023,2.1114395265,2.5787295234

B3LYP/6-31+G*
E(RB3LYP) = -219.761728861

Zero-point correction= 0.116772 (Hartree/Particle)
Thermal correction to Energy= 0.122883
Thermal correction to Enthalpy= 0.123827
Thermal correction to Gibbs Free Energy= 0.087856
Sum of electronic and zero-point Energies= -219.644956
Sum of electronic and thermal Energies= -219.638846
Sum of electronic and thermal Enthalpies= -219.637902
Sum of electronic and thermal Free Energies= -219.673872

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.110	21.814	75.707

O,0,2.3478542637,0.5716661201,1.2788446001
C,0,2.6950841237,-0.4076374744,2.1440855432
C,0,2.0380250452,-0.7482020271,3.3620648486

H,0,1.1528788656,-0.1901478389,3.6450720579
C,0,1.4186844477,1.5764256364,1.707201236
B,0,3.486517056,-0.010541054,3.8570107323
H,0,3.2966020718,-1.1541676171,1.6356592125
H,0,4.071806945,0.2831081859,2.7859554277
H,0,3.2540145387,1.0497238853,4.3665988233
H,0,4.2345185995,-0.8099486913,4.346311012
H,0,1.995685863,-1.8053751394,3.6016076281
H,0,1.3362110779,2.2678954106,0.8688172256
H,0,0.4380527238,1.1380996828,1.9197647058
H,0,1.7968973783,2.1035189213,2.5875159468

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.112904	E(Thermal)=	0.119129
E(QCISD(T))=	-219.032600	E(Empiric)=	-0.101400
DE(Plus)=	-0.014195	DE(2DF)=	-0.210595
E(Delta-G3)=	-0.292933	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.538819	G3 Energy=	-219.532594
G3 Enthalpy=	-219.531650	G3 Free Energy=	-219.567829

For Anharmonic Corrections of 6c-5

Zero-point vibrational energy 308783.1 (Joules/Mol)
73.80092 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 180.02 258.41 359.10 478.87 640.30
(Kelvin) 797.56 1032.91 1073.11 1130.62 1290.45
1344.54 1474.42 1494.26 1545.31 1660.58
1691.46 1700.90 1746.46 1779.78 1817.42
1915.28 2070.03 2164.71 2191.47 2204.10
2214.06 3214.80 3676.66 3816.07 4398.84
4506.81 4557.50 4567.33 4617.01 4664.87

Zero-point correction=	0.117609 (Hartree/Particle)
Thermal correction to Energy=	0.123658
Thermal correction to Enthalpy=	0.124603
Thermal correction to Gibbs Free Energy=	0.088734
Sum of electronic and zero-point Energies=	-219.623473
Sum of electronic and thermal Energies=	-219.617423
Sum of electronic and thermal Enthalpies=	-219.616479
Sum of electronic and thermal Free Energies=	-219.652347

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	77.597	21.525	75.491

ZPE(harm) = 0.30878D+03 kJ/mol ZPE(anh)= 0.30440D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.76921D-53	0.50606D-52	
QZvib	0.96035D+01	0.10788D+02	
Energy	0.32466D+03	0.32062D+03	kJ/mol
Enthalpy	0.32714D+03	0.32310D+03	kJ/mol
Entropy	0.32417D+03	0.32628D+03	J/(mol K)
Sp.Heat(V)	0.90059D+02	0.91856D+02	J/(mol K)
Sp.Heat(P)	0.98373D+02	0.10017D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.76921D-53	0.50606D-52	
QZvib	0.96035D+01	0.10788D+02	
Energy	0.32466D+03	0.32062D+03	kJ/mol
Enthalpy	0.32714D+03	0.32310D+03	kJ/mol
Entropy	0.32417D+03	0.32628D+03	J/(mol K)
Sp.Heat(V)	0.90059D+02	0.91856D+02	J/(mol K)
Sp.Heat(P)	0.98373D+02	0.10017D+03	J/(mol K)

6c-6 Transition State

B3LYP/6-31+G**

E(RB3LYP) = -219.755488581

Zero-point correction= 0.116408 (Hartree/Particle)
Thermal correction to Energy= 0.122477
Thermal correction to Enthalpy= 0.123421
Thermal correction to Gibbs Free Energy= 0.087654
Sum of electronic and ZPE= -219.639081
Sum of electronic and thermal Energies= -219.633012
Sum of electronic and thermal Enthalpies= -219.632068
Sum of electronic and thermal Free Energies= -219.667834

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	76.855	21.970	75.277

H,0,1.9552235842,0.6171509426,1.3250736661

C,0,2.4754990508,-0.1932845818,1.8255621166
C,0,1.8663961997,-0.7984040649,2.9415925619
O,0,0.5822832954,-0.3745053891,3.2649417061
B,0,3.1889943386,0.2026932878,3.4522459921
H,0,3.1931706047,-0.7475229668,1.2320911768
H,0,3.5967498541,0.8555109299,2.4701948759
H,0,2.6912759733,1.0571411124,4.1229564534
H,0,4.1071401351,-0.4778524367,3.800940077
H,0,2.078085622,-1.8421613763,3.1705506793
C,0,0.2324657771,-0.5717266601,4.6301750029
H,0,-0.8086369325,-0.2602912745,4.7323822233
H,0,0.322456059,-1.6305123555,4.912233976
H,0,0.8683614384,0.0323498329,5.2891374927

B3LYP/6-31G*
E(RB3LYP) = -219.734161161

Zero-point correction= 0.117267 (Hartree/Particle)
Thermal correction to Energy= 0.123272
Thermal correction to Enthalpy= 0.124216
Thermal correction to Gibbs Free Energy= 0.088576
Sum of electronic and ZPE= -219.616894
Sum of electronic and thermal Energies= -219.610889
Sum of electronic and thermal Enthalpies= -219.609945
Sum of electronic and thermal Free Energies= -219.645586

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	77.354	21.694	75.012

H,0,1.9533335972,0.6194716334,1.3297994925
C,0,2.478073862,-0.1892664423,1.829570285
C,0,1.8681165932,-0.7988895627,2.9471936293
O,0,0.5818345165,-0.3795904688,3.2613494618
B,0,3.1790846681,0.1962948717,3.4623981744
H,0,3.1918949563,-0.7426170528,1.2293075406
H,0,3.5881218473,0.8414449785,2.4680731751
H,0,2.6919046045,1.0655825377,4.1232143528
H,0,4.1064693557,-0.4755454897,3.8049929943
H,0,2.077230145,-1.8474214609,3.1607656196
C,0,0.2374547394,-0.5701424866,4.6242000856
H,0,-0.8045289412,-0.2588281537,4.729322931
H,0,0.3273407206,-1.6274502353,4.9165472604
H,0,0.8731343354,0.0355423314,5.2833429977

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.112577	E(Thermal)=	0.118761
E(QCISD(T))=	-219.026142	E(Empiric)=	-0.101400
DE(Plus)=	-0.015295	DE(2DF)=	-0.209233
E(Delta-G3)=	-0.292587	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.532080	G3 Energy=	-219.525896
G3 Enthalpy=	-219.524952	G3 Free Energy=	-219.560905

For Anharmonic Corrections of 6c-6

Zero-point vibrational energy 307886.8 (Joules/Mol)
73.58672 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 204.90 308.89 358.39 524.55 641.06
(Kelvin) 714.44 923.12 1041.27 1135.51 1251.23
1440.04 1497.06 1510.44 1581.03 1620.18
1686.53 1704.51 1717.55 1727.39 1819.30
1867.64 2053.75 2153.13 2180.62 2207.34
2221.23 3303.94 3716.10 3868.08 4334.77
4425.63 4515.90 4528.63 4571.60 4704.70

Zero-point correction= 0.117268 (Hartree/Particle)
Thermal correction to Energy= 0.123272
Thermal correction to Enthalpy= 0.124216
Thermal correction to Gibbs Free Energy= 0.088576
Sum of electronic and zero-point Energies= -219.616893
Sum of electronic and thermal Energies= -219.610889
Sum of electronic and thermal Enthalpies= -219.609945
Sum of electronic and thermal Free Energies= -219.645585

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.355	21.694	75.012

ZPE(harm) = 0.30789D+03 kJ/mol ZPE(anh)= 0.30301D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.91030D-53	0.77011D-52	
QZvib	0.79169D+01	0.93590D+01	
Energy	0.32365D+03	0.31917D+03	kJ/mol
Enthalpy	0.32613D+03	0.32165D+03	kJ/mol
Entropy	0.32216D+03	0.32488D+03	J/(mol K)

Sp.Heat(V)	0.90767D+02	0.92950D+02	J/(mol K)
Sp.Heat(P)	0.99082D+02	0.10126D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.91030D-53	0.77011D-52	
QZvib	0.79169D+01	0.93590D+01	
Energy	0.32365D+03	0.31917D+03	kJ/mol
Enthalpy	0.32613D+03	0.32165D+03	kJ/mol
Entropy	0.32216D+03	0.32488D+03	J/(mol K)
Sp.Heat(V)	0.90767D+02	0.92950D+02	J/(mol K)
Sp.Heat(P)	0.99082D+02	0.10126D+03	J/(mol K)

6c-7 Transition State

B3LYP/6-31+G**

E(RB3LYP) = -219.765592338

Zero-point correction= 0.116833 (Hartree/Particle)
Thermal correction to Energy= 0.123991
Thermal correction to Enthalpy= 0.124936
Thermal correction to Gibbs Free Energy= 0.086711
Sum of electronic and zero-point Energies= -219.648759
Sum of electronic and thermal Energies= -219.641601
Sum of electronic and thermal Enthalpies= -219.640657
Sum of electronic and thermal Free Energies= -219.678881

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.806	24.734	80.451

O,0,2.1038392358,0.4872833917,1.2615389779
C,0,2.3783763042,-0.5209409822,2.0838189085
C,0,1.9559772937,-0.7043921025,3.3733696631
H,0,1.2034957466,-0.0682022156,3.8223823235
C,0,1.2570301645,1.5462621046,1.7347674927
B,0,3.7048984978,0.0636449503,3.8571436235
H,0,3.0349242295,-1.2376440519,1.6007932642
H,0,3.8165955838,1.1364353276,3.3241018038
H,0,3.3897805714,0.107469526,5.0194820254
H,0,4.5304940667,-0.7641257441,3.5792694321
H,0,2.0847423959,-1.6867801261,3.8100949661

H,0,1.1836484099,2.252610304,0.9089731233
H,0,0.2643563808,1.1596486189,1.9878065118
H,0,1.7147191194,2.0263909993,2.604249884

B3LYP/6-31+G*
E(RB3LYP) = -219.745976528

Zero-point correction= 0.117745 (Hartree/Particle)
Thermal correction to Energy= 0.124817
Thermal correction to Enthalpy= 0.125761
Thermal correction to Gibbs Free Energy= 0.087758
Sum of electronic and zero-point Energies= -219.628232
Sum of electronic and thermal Energies= -219.621160
Sum of electronic and thermal Enthalpies= -219.620216
Sum of electronic and thermal Free Energies= -219.658219

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.324	24.488	79.984

O,0,2.1054790875,0.4857381732,1.2605066581
C,0,2.3795527188,-0.5186428174,2.084832965
C,0,1.9576485082,-0.7058775577,3.3738663673
H,0,1.2004584575,-0.0726707211,3.8207467862
C,0,1.2648635882,1.543404719,1.7385904026
B,0,3.6956775904,0.0648979167,3.8507351352
H,0,3.037385044,-1.2353444949,1.6028128708
H,0,3.813572619,1.1365047001,3.3136794902
H,0,3.376443395,0.1187737038,5.0126244385
H,0,4.5246902766,-0.7632460214,3.5820650156
H,0,2.0813122259,-1.6906970148,3.8076463749
H,0,1.1779333238,2.2465560653,0.9104026028
H,0,0.2750956805,1.159325296,2.0091186621
H,0,1.7327654846,2.0289380532,2.6001642305

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.113035 E(Thermal)= 0.120297
E(QCISD(T))= -219.036550 E(Empiric)= -0.101400
DE(Plus)= -0.013892 DE(2DF)= -0.210401
E(Delta-G3)= -0.293529 E(G3-Empiric)= -0.101400
G3(0 K)= -219.542738 G3 Energy= -219.535475

G3 Enthalpy= -219.534531 G3 Free Energy= -219.572902

For Anharmonic Corrections of 6c-7

Zero-point vibrational energy 309142.2 (Joules/Mol)
73.88677 (Kcal/Mol)
Warning -- explicit consideration of 8 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 134.13 229.93 294.73 322.86 446.33
(Kelvin) 460.19 615.08 866.31 1052.65 1089.24
1300.00 1328.26 1351.66 1446.71 1511.03
1611.43 1689.15 1702.86 1726.78 1769.28
1842.22 1979.68 2093.69 2161.68 2188.24
2203.51 2375.02 3617.75 3721.24 3757.80
4401.53 4514.12 4583.63 4601.76 4647.60
4724.34

Zero-point correction= 0.117746 (Hartree/Particle)
Thermal correction to Energy= 0.124817
Thermal correction to Enthalpy= 0.125761
Thermal correction to Gibbs Free Energy= 0.087764
Sum of electronic and zero-point Energies= -219.628230
Sum of electronic and thermal Energies= -219.621160
Sum of electronic and thermal Enthalpies= -219.620215
Sum of electronic and thermal Free Energies= -219.658213

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.324	24.487	79.972

ZPE(harm) = 0.30914D+03 kJ/mol ZPE(anh)= 0.30353D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.19356D-52	0.77920D-52	
QZvib	0.27933D+02	0.11685D+02	
Energy	0.32771D+03	0.32051D+03	kJ/mol
Enthalpy	0.33019D+03	0.32299D+03	kJ/mol
Entropy	0.33460D+03	0.33036D+03	J/(mol K)
Sp.Heat(V)	0.10245D+03	0.96241D+02	J/(mol K)
Sp.Heat(P)	0.11077D+03	0.10456D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.19356D-52	0.77920D-52	
QZvib	0.27933D+02	0.11685D+02	
Energy	0.32771D+03	0.32051D+03	kJ/mol
Enthalpy	0.33019D+03	0.32299D+03	kJ/mol
Entropy	0.33460D+03	0.33036D+03	J/(mol K)
Sp.Heat(V)	0.10245D+03	0.96241D+02	J/(mol K)
Sp.Heat(P)	0.11077D+03	0.10456D+03	J/(mol K)

6c-8 Complex
B3LYP/6-31+G**
E(RB3LYP) = -219.746226398

Zero-point correction= 0.117563 (Hartree/Particle)
Thermal correction to Energy= 0.124561
Thermal correction to Enthalpy= 0.125505
Thermal correction to Gibbs Free Energy= 0.087556
Sum of electronic and zero-point Energies= -219.628663
Sum of electronic and thermal Energies= -219.621666
Sum of electronic and thermal Enthalpies= -219.620721
Sum of electronic and thermal Free Energies= -219.658670

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	78.163	24.190	79.870

H,0,2.0365150571,0.4537368746,1.3165225076
C,0,2.4861989543,-0.3131050877,1.9369086559
C,0,1.7541418771,-0.8118660671,2.9934672214
O,0,0.5482933099,-0.3180191493,3.2917917983
B,0,3.3169461501,0.4664349847,3.3905517623
H,0,3.2288702933,-0.9488817914,1.4717898889
H,0,3.1681980991,1.6244425293,3.1052473389
H,0,2.7807151804,0.2665094531,4.4682636052
H,0,4.4061495888,-0.040638264,3.3903916893
H,0,2.064341996,-1.7090667538,3.5283596098
C,0,0.0767361983,-0.5671601111,4.6195171363
H,0,-0.9636787576,-0.2414021562,4.6400436994
H,0,0.1351258567,-1.6359370627,4.8608269025
H,0,0.6692971965,0.0076856015,5.3390311843

B3LYP/6-31+G*
E(RB3LYP) = -219.746226398

Zero-point correction= 0.117563 (Hartree/Particle)
Thermal correction to Energy= 0.124561
Thermal correction to Enthalpy= 0.125505
Thermal correction to Gibbs Free Energy= 0.087556
Sum of electronic and zero-point Energies= -219.628663
Sum of electronic and thermal Energies= -219.621666
Sum of electronic and thermal Enthalpies= -219.620721
Sum of electronic and thermal Free Energies= -219.658670

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.163	24.190	79.870

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.112862	E(Thermal)=	0.120048
E(QCISD(T))=	-219.036893	E(Empiric)=	-0.101400
DE(Plus)=	-0.014225	DE(2DF)=	-0.209222
E(Delta-G3)=	-0.293342	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.542220	G3 Energy=	-219.535034
G3 Enthalpy=	-219.534089	G3 Free Energy=	-219.572405

For Anharmonic Corrections of 6c-8
Zero-point vibrational energy 308665.1 (Joules/Mol)
73.77272 (Kcal/Mol)
Warning -- explicit consideration of 8 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 130.55 189.36 267.28 393.99 407.76
(Kelvin) 549.96 731.10 768.71 1076.07 1160.66
1279.15 1302.99 1428.70 1478.14 1588.21
1630.47 1677.94 1700.90 1709.11 1719.19
1863.06 1920.10 2092.65 2160.06 2181.07
2199.35 2349.14 3515.44 3660.77 3787.67
4382.81 4488.77 4560.57 4574.00 4596.21
4725.77

Zero-point correction= 0.117564 (Hartree/Particle)
Thermal correction to Energy= 0.124563
Thermal correction to Enthalpy= 0.125507
Thermal correction to Gibbs Free Energy= 0.087554
Sum of electronic and zero-point Energies= -219.628662

Sum of electronic and thermal Energies= -219.621664
Sum of electronic and thermal Enthalpies= -219.620720
Sum of electronic and thermal Free Energies= -219.658672

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.164	24.190	79.878

ZPE(harm) = 0.30867D+03 kJ/mol ZPE(anh)= 0.30363D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.24680D-52	0.30804D-51	
QZvib	0.29380D+02	0.48173D+02	
Energy	0.32704D+03	0.32282D+03	kJ/mol
Enthalpy	0.32952D+03	0.32530D+03	kJ/mol
Entropy	0.33421D+03	0.34105D+03	J/(mol K)
Sp.Heat(V)	0.10121D+03	0.10433D+03	J/(mol K)
Sp.Heat(P)	0.10953D+03	0.11264D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.24680D-52	0.30804D-51	
QZvib	0.29380D+02	0.48173D+02	
Energy	0.32704D+03	0.32282D+03	kJ/mol
Enthalpy	0.32952D+03	0.32530D+03	kJ/mol
Entropy	0.33421D+03	0.34105D+03	J/(mol K)
Sp.Heat(V)	0.10121D+03	0.10433D+03	J/(mol K)
Sp.Heat(P)	0.10953D+03	0.11264D+03	J/(mol K)

6c-9 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -219.794184065

Zero-point correction= 0.119516 (Hartree/Particle)
Thermal correction to Energy= 0.126077
Thermal correction to Enthalpy= 0.127022
Thermal correction to Gibbs Free Energy= 0.090405
Sum of electronic and ZPE= -219.674668
Sum of electronic and thermal Energies= -219.668107
Sum of electronic and thermal Enthalpies= -219.667162
Sum of electronic and thermal Free Energies= -219.703779

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	79.115	23.412	77.065

C,0,2.3280035036,-0.864199454,3.7178243312
C,0,2.0488743314,-0.5954102753,2.2618401515
O,0,2.5453172932,0.7865658847,1.8619632582
C,0,1.6096795028,1.6405872758,1.1851421851
B,0,3.1173956433,-0.607920101,1.1160572864
H,0,1.7123219944,-0.2522288161,4.3884605567
H,0,0.990968778,-0.6679301103,1.9997772308
H,0,4.2714019328,-0.7625155473,1.387447287
H,0,3.3826607189,-0.6956670602,3.9517085386
H,0,2.7534184318,-0.647955941,-0.024497413
H,0,2.1046092832,-1.9180322965,3.9248862069
H,0,2.188182315,2.454612684,0.7432297549
H,0,1.0818068036,1.0937117289,0.3977855154
H,0,0.8993394679,2.036963028,1.9171241103

B3LYP/6-31G*
E(RB3LYP) = -219.775347862

Zero-point correction= 0.120488 (Hartree/Particle)
Thermal correction to Energy= 0.126979
Thermal correction to Enthalpy= 0.127924
Thermal correction to Gibbs Free Energy= 0.091460
Sum of electronic and ZPE= -219.654860
Sum of electronic and thermal Energies= -219.648368
Sum of electronic and thermal Enthalpies= -219.647424
Sum of electronic and thermal Free Energies= -219.683888

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	79.681	23.186	76.745

C,0,2.3275932655,-0.8631329665,3.7160308419
C,0,2.0485646196,-0.59459215,2.2598235245
O,0,2.5482147121,0.7867811505,1.8670599183
C,0,1.6124831378,1.6333315451,1.1874570513
B,0,3.1164039877,-0.6037141474,1.1145024109
H,0,1.7176704608,-0.2437816453,4.3866042827
H,0,0.9893559586,-0.6634092583,2.0010394861
H,0,4.2709673035,-0.7604463263,1.3852725921
H,0,3.3843988311,-0.7014161167,3.9487113736

H,0,2.7504001621,-0.6401793325,-0.0263541099
H,0,2.096253543,-1.9145866393,3.9282202724
H,0,2.1870616596,2.4526474195,0.7488049561
H,0,1.0896748611,1.0864347189,0.3963937104
H,0,0.8949374974,2.0266447483,1.9151826897

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.115668	E(Thermal)=	0.122349
E(QCISD(T))=	-219.071551	E(Empiric)=	-0.101400
DE(Plus)=	-0.013136	DE(2DF)=	-0.208248
E(Delta-G3)=	-0.292143	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.570809	G3 Energy=	-219.564129
G3 Enthalpy=	-219.563185	G3 Free Energy=	-219.599991

6c-10 Product
B3LYP/6-31+G**
E(RB3LYP) = -219.792276638

Zero-point correction= 0.117930 (Hartree/Particle)
Thermal correction to Energy= 0.125140
Thermal correction to Enthalpy= 0.126084
Thermal correction to Gibbs Free Energy= 0.087215
Sum of electronic and ZPE= -219.674347
Sum of electronic and thermal Energies= -219.667137
Sum of electronic and thermal Enthalpies= -219.666193
Sum of electronic and thermal Free Energies= -219.705061

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	78.526	23.884	81.806

O,0,1.906052732,0.198370954,1.1485633587
C,0,2.8911118272,-0.0735002293,2.1417932141
C,0,2.3259936413,-0.3395487835,3.5401125789
H,0,1.7965698164,0.5557827981,3.9223320356
C,0,1.325536975,1.4864559575,1.2357677335
B,0,3.353346294,-0.6435948186,4.6739781255
H,0,3.4170957176,-0.9617308846,1.7779004459
H,0,3.6211816338,0.7519494551,2.1779872596
H,0,2.9698587712,-1.0524778589,5.7308368621
H,0,4.5258119549,-0.4364784511,4.536477848
H,0,1.5414610643,-1.1091610903,3.4973542336

H,0,0.6633971077,1.5953653966,0.373716168
H,0,0.7310936066,1.618496131,2.1517312254
H,0,2.0943218584,2.2744894238,1.1979579109

B3LYP/6-31G*
E(RB3LYP) = -219.770912998

Zero-point correction= 0.118831 (Hartree/Particle)
Thermal correction to Energy= 0.125970
Thermal correction to Enthalpy= 0.126914
Thermal correction to Gibbs Free Energy= 0.088287
Sum of electronic and ZPE= -219.652082
Sum of electronic and thermal Energies= -219.644943
Sum of electronic and thermal Enthalpies= -219.643999
Sum of electronic and thermal Free Energies= -219.682626

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	79.047	23.682	81.298

O,0,1.9021319184,0.193309213,1.1485273636
C,0,2.8860296838,-0.0809207572,2.1354764612
C,0,2.3215085529,-0.3426410848,3.5362651777
H,0,1.8008101777,0.5618152661,3.912036675
C,0,1.3334579056,1.4809776266,1.2429395895
B,0,3.3505853346,-0.6362358846,4.6720551762
H,0,3.4069670211,-0.9737061234,1.7734083001
H,0,3.6246960059,0.7377265313,2.1741127149
H,0,2.9793036652,-1.0879326839,5.7168566946
H,0,4.5141429565,-0.371966427,4.5503113834
H,0,1.5296455831,-1.1040777259,3.4928257055
H,0,0.6661224297,1.5982835422,0.3847149948
H,0,0.7435220881,1.6207679222,2.1623588102
H,0,2.1039096774,2.2690185852,1.2046199533

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.114078	E(Thermal)=	0.121389
E(QCISD(T))=	-219.063124	E(Empiric)=	-0.101400
DE(Plus)=	-0.014990	DE(2DF)=	-0.207704
E(Delta-G3)=	-0.293170	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.566311	G3 Energy=	-219.559000
G3 Enthalpy=	-219.558056	G3 Free Energy=	-219.597034

6c-11 Product
B3LYP/6-31+G**
E(RB3LYP) = -219.789548489

Zero-point correction= 0.117883 (Hartree/Particle)
Thermal correction to Energy= 0.125017
Thermal correction to Enthalpy= 0.125961
Thermal correction to Gibbs Free Energy= 0.087850
Sum of electronic and ZPE= -219.671665
Sum of electronic and thermal Energies= -219.664532
Sum of electronic and thermal Enthalpies= -219.663587
Sum of electronic and thermal Free Energies= -219.701699

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	78.449	24.320	80.212

H,0,1.6614141253,-0.4249097911,0.9801361
C,0,2.4576029243,-0.0985999942,1.6561587476
C,0,2.1001683851,-0.514751371,3.099751974
O,0,0.7806219976,-0.0064521926,3.3542899343
B,0,3.2283719499,0.0008459252,4.0604322785
H,0,3.4003326946,-0.5533145088,1.3385407631
H,0,2.544864194,0.9893217493,1.5663018265
H,0,3.0306215139,0.8573854146,4.8694786449
H,0,4.331217515,-0.4471712844,3.9411188226
H,0,2.0641147102,-1.6223545577,3.1198160432
C,0,0.2143946497,-0.4865503142,4.5569011349
H,0,-0.7784078397,-0.0394108732,4.6476039432
H,0,0.1121234773,-1.5841310635,4.5428873529
H,0,0.8120247028,-0.2013221385,5.4366604342

B3LYP/6-31G*
E(RB3LYP) = -219.768510929

Zero-point correction= 0.118793 (Hartree/Particle)
Thermal correction to Energy= 0.125885
Thermal correction to Enthalpy= 0.126829
Thermal correction to Gibbs Free Energy= 0.088820
Sum of electronic and ZPE= -219.649718
Sum of electronic and thermal Energies= -219.642626
Sum of electronic and thermal Enthalpies= -219.641682
Sum of electronic and thermal Free Energies= -219.679691

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	78.994	24.135	79.997

H,0,1.6552414185,-0.4153991883,0.9874794812
C,0,2.4569261528,-0.0988800796,1.6624572735
C,0,2.0961282364,-0.5196217907,3.1050651528
O,0,0.7839060739,-0.0023722982,3.3570108642
B,0,3.2275446586,0.0064304246,4.0570208199
H,0,3.3956409101,-0.558973844,1.3393044422
H,0,2.5518447441,0.9893181986,1.5770535544
H,0,3.0370307896,0.8957751647,4.8334749423
H,0,4.3271989127,-0.457631659,3.9622080902
H,0,2.0592003632,-1.6269555705,3.121604482
C,0,0.2179843581,-0.4914642752,4.5504768024
H,0,-0.7706251522,-0.0350281539,4.6521228999
H,0,0.1021747538,-1.5888547004,4.5284162676
H,0,0.8192687803,-0.2277572282,5.4363829273

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.114041	E(Thermal)=	0.121315
E(QCISD(T))=	-219.061676	E(Empiric)=	-0.101400
DE(Plus)=	-0.015057	DE(2DF)=	-0.207680
E(Delta-G3)=	-0.292891	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.564662	G3 Energy=	-219.557388
G3 Enthalpy=	-219.556444	G3 Free Energy=	-219.594813

6c-12 Product
B3LYP/6-31+G**
E(RB3LYP) = -219.794376253

Zero-point correction= 0.118111 (Hartree/Particle)
Thermal correction to Energy= 0.125189
Thermal correction to Enthalpy= 0.126133
Thermal correction to Gibbs Free Energy= 0.087787
Sum of electronic and ZPE= -219.676265
Sum of electronic and thermal Energies= -219.669188
Sum of electronic and thermal Enthalpies= -219.668244
Sum of electronic and thermal Free Energies= -219.706589

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 78.557 23.690 80.706

C,0,2.748350236,-0.570650805,2.0855497371
B,0,3.5466685115,0.7200161767,2.4645665256
C,0,1.7823174236,-1.0832287865,3.1464223691
O,0,0.7889835544,-0.0817755661,3.3418092299
C,0,-0.1624702531,-0.4246927492,4.3315913482
H,0,2.2379691644,-0.4763931202,1.118315799
H,0,3.5344664134,-1.3328210541,1.9179941803
H,0,3.7536417345,0.9970120965,3.6109046731
H,0,2.3136991574,-1.2696534597,4.0949759079
H,0,4.0328905187,1.4077412139,1.6139108691
H,0,1.2993613733,-2.0268908017,2.841758592
H,0,-0.8727349529,0.4025578559,4.3975810376
H,0,-0.7064733358,-1.3444037609,4.0652431411
H,0,0.3134684548,-0.5696362397,5.3138785901

B3LYP/6-31G*
E(RB3LYP) = -219.773104612

Zero-point correction= 0.119088 (Hartree/Particle)
Thermal correction to Energy= 0.126139
Thermal correction to Enthalpy= 0.127083
Thermal correction to Gibbs Free Energy= 0.088681
Sum of electronic and ZPE= -219.654017
Sum of electronic and thermal Energies= -219.646966
Sum of electronic and thermal Enthalpies= -219.646022
Sum of electronic and thermal Free Energies= -219.684424

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 79.153 23.444 80.824

C,0,2.7603160102,-0.5967071873,2.0820638714
B,0,3.5050923973,0.7233707261,2.4800562043
C,0,1.7839164312,-1.1006557473,3.1385029955
O,0,0.8153632082,-0.079369647,3.3291363033
C,0,-0.1369557667,-0.4009437848,4.3189778905
H,0,2.2602616865,-0.5217524311,1.1082159964
H,0,3.5608386957,-1.34855284,1.9439506457
H,0,3.7562248495,0.9526415305,3.6290859423
H,0,2.312753267,-1.3020808849,4.0859778325
H,0,3.9058688444,1.4853410346,1.6472514381

H,0,1.2875320407,-2.037635667,2.8313571427
H,0,-0.8310865252,0.4410124289,4.3871078239
H,0,-0.7036495891,-1.310176784,4.0594964804
H,0,0.3336624504,-0.5573097466,5.3033214331

E(ZPE)=	0.114324	E(Thermal)=	0.121546
E(QCISD(T))=	-219.066203	E(Empiric)=	-0.101400
DE(Plus)=	-0.014982	DE(2DF)=	-0.207509
E(Delta-G3)=	-0.292954	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.568724	G3 Energy=	-219.561502
G3 Enthalpy=	-219.560558	G3 Free Energy=	-219.599307

For Anharmonic Corrections of 6c-8

Zero-point vibrational energy 308013.1 (Joules/Mol)
73.61690 (Kcal/Mol)
Warning -- explicit consideration of 6 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 202.88 260.46 373.86 426.72 678.85
(Kelvin) 762.23 1004.53 1090.59 1128.44 1306.91
1341.63 1481.46 1516.79 1587.58 1661.94
1691.54 1695.46 1708.37 1765.26 1847.60
1878.55 2073.53 2155.87 2182.78 2195.57
2236.53 3192.56 3676.66 3826.32 4365.14
4457.47 4518.13 4557.23 4567.16 4674.23

Zero-point correction= 0.117316 (Hartree/Particle)
Thermal correction to Energy= 0.123357
Thermal correction to Enthalpy= 0.124301
Thermal correction to Gibbs Free Energy= 0.088479
Sum of electronic and zero-point Energies= -219.627108
Sum of electronic and thermal Energies= -219.621067
Sum of electronic and thermal Enthalpies= -219.620123
Sum of electronic and thermal Free Energies= -219.655944

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.408	21.540	75.393

ZPE(harm) = 0.30801D+03 kJ/mol ZPE(anh)= 0.30324D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value
Qvib	0.98066D-53	0.10668D-51
QZvib	0.89747D+01	0.14244D+02

Energy	0.32387D+03	0.31974D+03	kJ/mol
Enthalpy	0.32635D+03	0.32221D+03	kJ/mol
Entropy	0.32376D+03	0.32972D+03	J/(mol K)
Sp.Heat(V)	0.90123D+02	0.92403D+02	J/(mol K)
Sp.Heat(P)	0.98438D+02	0.10072D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.98066D-53	0.10668D-51	
QZvib	0.89747D+01	0.14244D+02	
Energy	0.32387D+03	0.31974D+03	kJ/mol
Enthalpy	0.32635D+03	0.32221D+03	kJ/mol
Entropy	0.32376D+03	0.32972D+03	J/(mol K)
Sp.Heat(V)	0.90123D+02	0.92403D+02	J/(mol K)
Sp.Heat(P)	0.98438D+02	0.10072D+03	J/(mol K)

6c-13 Variational Transition State

B3LYP/6-31+G**
E(RB3LYP) = -219.752348645

Zero-point correction= 0.112705 (Hartree/Particle)
Thermal correction to Energy= 0.120277
Thermal correction to Enthalpy= 0.121221
Thermal correction to Gibbs Free Energy= 0.080275
Sum of electronic and zero-point Energies= -219.639644
Sum of electronic and thermal Energies= -219.632071
Sum of electronic and thermal Enthalpies= -219.631127
Sum of electronic and thermal Free Energies= -219.672074

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.475	24.082	86.179

B3LYP/6-31+G*
E(RB3LYP) = -219.730356621

Zero-point correction= 0.113315 (Hartree/Particle)
Thermal correction to Energy= 0.120967
Thermal correction to Enthalpy= 0.121911
Thermal correction to Gibbs Free Energy= 0.080355
Sum of electronic and ZPE= -219.617042
Sum of electronic and thermal Energies= -219.609390

Sum of electronic and thermal Enthalpies= -219.608446
Sum of electronic and thermal Free Energies= -219.650001

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	75.908	24.044	87.461

C,0,-0.35337,0.64905,0.62194
C,0,-0.06192,1.36296,-0.47443
H,0,-0.38523,1.09034,-1.47268
C,0,-1.5708,-1.04237,-0.49648
B,0,3.18495,-0.31874,-0.12988
H,0,-0.02635,0.95733,1.61134
H,0,3.6737,0.7662,-0.22875
H,0,2.95695,-0.77516,0.94949
H,0,2.96536,-0.96536,-1.10956
H,0,0.50708,2.27859,-0.36808
H,0,-2.09415,-1.9603,-0.22416
H,0,-2.27028,-0.34633,-0.97759
H,0,-0.75644,-1.27392,-1.19518
O,0,-1.06437,-0.49923,0.71571

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.108782	E(Thermal)=	0.116592
E(QCISD(T))=	-219.021679	E(Empiric)=	-0.101400
DE(Plus)=	-0.015577	DE(2DF)=	-0.206594
E(Delta-G3)=	-0.293368	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.529836	G3 Energy=	-219.522026
G3 Enthalpy=	-219.521082	G3 Free Energy=	-219.562995

6c-14 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -219.750269066

Zero-point correction= 0.112402 (Hartree/Particle)
Thermal correction to Energy= 0.120924
Thermal correction to Enthalpy= 0.121868
Thermal correction to Gibbs Free Energy= 0.078920
Sum of electronic and zero-point Energies= -219.637867
Sum of electronic and thermal Energies= -219.629345
Sum of electronic and thermal Enthalpies= -219.628401
Sum of electronic and thermal Free Energies= -219.671349

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	75.881	26.312	90.391

B3LYP/6-31+G*
E(RB3LYP) = -219.728383587

Zero-point correction= 0.112951 (Hartree/Particle)
Thermal correction to Energy= 0.121583
Thermal correction to Enthalpy= 0.122527
Thermal correction to Gibbs Free Energy= 0.078612
Sum of electronic and ZPE= -219.615433
Sum of electronic and thermal Energies= -219.606800
Sum of electronic and thermal Enthalpies= -219.605856
Sum of electronic and thermal Free Energies= -219.649772

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	76.295	26.296	92.428

C,0,-0.59078,-1.70318,-0.13091
C,0,-0.60988,-0.45871,0.35904
O,0,-1.04105,0.60472,-0.36727
B,0,2.71619,-0.6287,-0.04709
H,0,-0.31486,-2.53254,0.50852
H,0,2.54238,0.47684,-0.46606
H,0,2.73316,-0.8224,1.13147
H,0,2.94324,-1.52188,-0.80488
H,0,-0.3232,-0.23682,1.38889
C,0,-0.59076,1.87311,0.09486
H,0,-1.11075,2.6248,-0.50185
H,0,-0.83604,2.0209,1.156
H,0,0.49243,1.98156,-0.04317
H,0,-0.86516,-1.90942,-1.15574

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.108433	E(Thermal)=	0.117226
E(QCISD(T))=	-219.019573	E(Empiric)=	-0.101400
DE(Plus)=	-0.015770	DE(2DF)=	-0.206496
E(Delta-G3)=	-0.293273	E(G3-Empiric)=	-0.101400
G3(0 K)=	-219.528080	G3 Energy=	-219.519286
G3 Enthalpy=	-219.518342	G3 Free Energy=	-219.562658

6c-15 Starting Material
B3LYP/6-31+G**
E(RB3LYP) = -232.453001159

Zero-point correction= 0.112560 (Hartree/Particle)
Thermal correction to Energy= 0.119130
Thermal correction to Enthalpy= 0.120075
Thermal correction to Gibbs Free Energy= 0.081320
Sum of electronic and ZPE= -232.340442
Sum of electronic and thermal Energies= -232.333871
Sum of electronic and thermal Enthalpies= -232.332927
Sum of electronic and thermal Free Energies= -232.371681

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	74.755	21.306	81.566

H,0,1.9903952502,0.2401476876,0.9916090285
C,0,2.4513588567,-0.4416577611,1.6981301037
C,0,1.950939695,-0.6225399753,2.9235575185
O,0,0.8394472587,0.0297988427,3.3657787323
H,0,3.3380674217,-0.9848222919,1.3954058453
H,0,2.4078297139,-1.3057590937,3.6399974514
C,0,0.4264824783,-0.2731314516,4.7048348666
C,0,-0.8149894937,0.5427617029,5.0147471256
H,0,0.2178845502,-1.3494280694,4.7872653318
H,0,1.2403722428,-0.0270237497,5.4017821351
H,0,-1.1560624865,0.3325773675,6.0338610147
H,0,-0.6044965944,1.6132300214,4.9327400031
H,0,-1.623267893,0.2957017706,4.3200648433

B3LYP/6-31+G*
E(RB3LYP) = -232.429908112

Zero-point correction= 0.113326 (Hartree/Particle)
Thermal correction to Energy= 0.119850
Thermal correction to Enthalpy= 0.120795
Thermal correction to Gibbs Free Energy= 0.082490
Sum of electronic and ZPE= -232.316582
Sum of electronic and thermal Energies= -232.310058
Sum of electronic and thermal Enthalpies= -232.309114
Sum of electronic and thermal Free Energies= -232.347418

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	75.207	21.150	80.619

H,0,2.1007832875,0.3700792087,1.0697056311
C,0,2.4709795179,-0.4167708982,1.718665244
C,0,1.9045833663,-0.6714321877,2.8983892704
O,0,0.8201135437,0.0137287612,3.3563029053
H,0,3.3152472479,-1.008151518,1.3847376244
H,0,2.2706065533,-1.4594853955,3.5585187462
C,0,0.4546356737,-0.2400267807,4.7141107518
C,0,-0.8197578534,0.530342236,5.0095539104
H,0,0.30127144,-1.3197390421,4.8617436075
H,0,1.2672515104,0.0780968806,5.383873006
H,0,-1.1311867913,0.3636370307,6.0464281652
H,0,-0.6628379428,1.6033871284,4.8616616636
H,0,-1.6277285532,0.2061895767,4.3460834742

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.108793	E(Thermal)=	0.115465
E(QCISD(T))=	-231.716872	E(Empiric)=	-0.101400
DE(Plus)=	-0.016364	DE(2DF)=	-0.206860
E(Delta-G3)=	-0.300840	E(G3-Empiric)=	-0.101400
G3(0 K)=	-232.233542	G3 Energy=	-232.226870
G3 Enthalpy=	-232.225926	G3 Free Energy=	-232.264532

6c-16 Starting Material
B3LYP/6-31+G**
E(RB3LYP) = -232.452284218

Zero-point correction= 0.112835 (Hartree/Particle)
Thermal correction to Energy= 0.119135
Thermal correction to Enthalpy= 0.120079
Thermal correction to Gibbs Free Energy= 0.083093
Sum of electronic and ZPE= -232.339449
Sum of electronic and thermal Energies= -232.333150
Sum of electronic and thermal Enthalpies= -232.332205
Sum of electronic and thermal Free Energies= -232.369192

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 74.758 21.187 77.844

H,0,1.6580159273,-0.233542553,0.9059298192
C,0,2.3845471404,-0.4930446564,1.6682960501
C,0,2.0885818856,-0.4217698673,2.9688810842
O,0,0.8841410532,0.0215077007,3.4271993319
H,0,3.3758705706,-0.8020514789,1.3600344058
H,0,2.8113174606,-0.6828640665,3.7438267936
C,0,0.5772120924,-0.271744266,4.7965255115
H,0,-0.1857971567,0.4585094514,5.0789889795
C,0,0.0637504865,-1.6946763936,4.9824582678
H,0,1.4666200236,-0.0883283703,5.416776325
H,0,-0.2059874844,-1.8630423349,6.0312754934
H,0,-0.8230218327,-1.8664952761,4.3648808997
H,0,0.8238848337,-2.4316508892,4.7033970381

B3LYP/6-31+G*
E(RB3LYP) = -232.429580380

Zero-point correction= 0.113620 (Hartree/Particle)
Thermal correction to Energy= 0.119881
Thermal correction to Enthalpy= 0.120825
Thermal correction to Gibbs Free Energy= 0.083924
Sum of electronic and ZPE= -232.315961
Sum of electronic and thermal Energies= -232.309700
Sum of electronic and thermal Enthalpies= -232.308755
Sum of electronic and thermal Free Energies= -232.345656

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 75.226 21.019 77.664

H,0,1.6519535047,-0.2455307603,0.9117026318
C,0,2.3785850066,-0.5018244509,1.6755724736
C,0,2.0842501585,-0.420621493,2.9731672896
O,0,0.882912697,0.0311715145,3.4306462108
H,0,3.3686137617,-0.8131775587,1.3639453487
H,0,2.8076234037,-0.6783022013,3.7498043569
C,0,0.5788450605,-0.2667925325,4.7948873034
H,0,-0.1870942697,0.459230628,5.0830911543
C,0,0.0696289416,-1.6919862185,4.9762312597
H,0,1.4658293887,-0.0844927026,5.4203151589
H,0,-0.2016043817,-1.8700434794,6.023453383

H,0,-0.8146286587,-1.863631589,4.3540882867
H,0,0.8342203871,-2.4231921565,4.6915651427

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.109075	E(Thermal)=	0.115492
E(QCISD(T))=	-231.716806	E(Empiric)=	-0.101400
DE(Plus)=	-0.016240	DE(2DF)=	-0.206949
E(Delta-G3)=	-0.300454	E(G3-Empiric)=	-0.101400
G3(0 K)=	-232.232774	G3 Energy=	-232.226356
G3 Enthalpy=	-232.225412	G3 Free Energy=	-232.262612

6c-17 Starting Material
B3LYP/6-31+G**
E(RB3LYP) = -232.452950187

Zero-point correction= 0.113553 (Hartree/Particle)
Thermal correction to Energy= 0.119586
Thermal correction to Enthalpy= 0.120530
Thermal correction to Gibbs Free Energy= 0.084577
Sum of electronic and ZPE= -232.339397
Sum of electronic and thermal Energies= -232.333364
Sum of electronic and thermal Enthalpies= -232.332420
Sum of electronic and thermal Free Energies= -232.368374

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	75.041	20.924	75.671

O,0,1.987341231,0.4726545378,1.3207475979
C,0,2.3665570377,-0.5979532289,2.0669874222
C,0,2.1353692932,-0.852360809,3.3623156336
H,0,1.5636529155,-0.205438082,4.0164833382
C,0,1.232363158,1.522433205,1.9445744185
H,0,2.9361604251,-1.2847679835,1.4471140267
H,0,2.5417418459,-1.7605026111,3.7911638751
H,0,1.4119147521,2.3979475003,1.3146413126
C,0,-0.2585387062,1.2083104722,2.008265922
H,0,1.6473573071,1.7307676944,2.938508651
H,0,-0.7971576939,2.0561285625,2.4465916722
H,0,-0.653560396,1.0337314735,1.0029340682
H,0,-0.4612151696,0.3225462689,2.615932062

B3LYP/6-31+G**
E(RB3LYP) = -232.430736162

Zero-point correction= 0.114370 (Hartree/Particle)
Thermal correction to Energy= 0.120353
Thermal correction to Enthalpy= 0.121298
Thermal correction to Gibbs Free Energy= 0.085464
Sum of electronic and ZPE= -232.316366
Sum of electronic and thermal Energies= -232.310383
Sum of electronic and thermal Enthalpies= -232.309439
Sum of electronic and thermal Free Energies= -232.345272

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	75.523	20.738	75.417

O,0,1.9935738956,0.4806600661,1.3181878827
C,0,2.3599697941,-0.5916257735,2.0671667205
C,0,2.1256840321,-0.8484800987,3.3584575744
H,0,1.5577596779,-0.198812777,4.0141018211
C,0,1.2381006,1.5239338521,1.9425951773
H,0,2.9274810558,-1.2811750306,1.446982974
H,0,2.5242955838,-1.7598375478,3.7889617125
H,0,1.4092711171,2.4025201018,1.3134044174
C,0,-0.2510496978,1.2014637964,2.0117682919
H,0,1.6527797183,1.7369160202,2.9363216207
H,0,-0.7973836844,2.0447107328,2.4502603196
H,0,-0.6463567576,1.0198209047,1.0072045239
H,0,-0.4421393351,0.3134027533,2.6208469641

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.109795	(Thermal)=	0.115941
E(QCISD(T))=	-231.718383	E(Empiric)=	-0.101400
DE(Plus)=	-0.015716	DE(2DF)=	-0.207374
E(Delta-G3)=	-0.300617	E(G3-Empiric)=	-0.101400
G3(0 K)=	-232.233696	G3 Energy=	-232.227550
G3 Enthalpy=	-232.226606	G3 Free Energy=	-232.262733

6c-18 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -259.073411569

Zero-point correction= 0.141348 (Hartree/Particle)
Thermal correction to Energy= 0.150873
Thermal correction to Enthalpy= 0.151817
Thermal correction to Gibbs Free Energy= 0.105996
Sum of electronic and zero-point Energies= -258.932064
Sum of electronic and thermal Energies= -258.922538
Sum of electronic and thermal Enthalpies= -258.921594
Sum of electronic and thermal Free Energies= -258.967416

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.674	30.935	96.439

B3LYP/6-31+G*
E(RB3LYP) = -259.048518142

Zero-point correction= 0.142117 (Hartree/Particle)
Thermal correction to Energy= 0.150838
Thermal correction to Enthalpy= 0.151783
Thermal correction to Gibbs Free Energy= 0.108027
Sum of electronic and ZPE= -258.906402
Sum of electronic and thermal Energies= -258.897680
Sum of electronic and thermal Enthalpies= -258.896736
Sum of electronic and thermal Free Energies= -258.940491

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	94.653	28.867	92.091

C,0,0.31069,0.8246,0.64446
C,0,0.57087,1.35749,-0.55972
H,0,0.15234,0.98903,-1.48928
C,0,-1.09729,-0.98134,-0.07946
B,0,3.43014,-0.45867,-0.28866
H,0,0.73179,1.25268,1.55082
H,0,4.0382,0.53752,-0.03484
H,0,3.03705,-1.15948,0.59451
H,0,3.27591,-0.7887,-1.42625
H,0,1.20787,2.23206,-0.61449
H,0,-1.23358,-1.98514,0.33312
C,0,-2.44275,-0.37145,-0.45617
H,0,-0.42782,-1.06245,-0.94435
H,0,-2.93122,-0.98504,-1.22198
H,0,-3.09802,-0.32753,0.41959

H,0,-2.32747,0.6427,-0.85032
O,0,-0.44772,-0.24755,0.96934

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.136432	E(Thermal)=	0.145362
E(QCISD(T))=	-258.208070	E(Empiric)=	-0.121680
DE(Plus)=	-0.016784	DE(2DF)=	-0.245983
E(Delta-G3)=	-0.349279	E(G3-Empiric)=	-0.121680
G3(0 K)=	-258.805364	G3 Energy=	-258.796434
G3 Enthalpy=	-258.795490	G3 Free Energy=	-258.839698

6c-19 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -259.074976007

Zero-point correction= 0.141326 (Hartree/Particle)
Thermal correction to Energy= 0.150753
Thermal correction to Enthalpy= 0.151698
Thermal correction to Gibbs Free Energy= 0.106221
Sum of electronic and zero-point Energies= -258.933650
Sum of electronic and thermal Energies= -258.924223
Sum of electronic and thermal Enthalpies= -258.923278
Sum of electronic and thermal Free Energies= -258.968755

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	94.599	30.832	95.713

B3LYP/6-31+G*
E(RB3LYP) = -259.050219227

Zero-point correction= 0.142154 (Hartree/Particle)
Thermal correction to Energy= 0.151655
Thermal correction to Enthalpy= 0.152599
Thermal correction to Gibbs Free Energy= 0.106447
Sum of electronic and ZPE= -258.908065
Sum of electronic and thermal Energies= -258.898564
Sum of electronic and thermal Enthalpies= -258.897620
Sum of electronic and thermal Free Energies= -258.943772

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 95.165 30.757 97.135

C,0,-0.99671,1.80594,0.02987
C,0,-0.28299,0.69469,0.26244
O,0,0.49873,0.11991,-0.68137
B,0,-3.1389,-0.39652,0.10067
H,0,-1.57489,2.25299,0.82909
H,0,-2.44894,-1.35824,-0.06937
H,0,-3.41037,-0.05282,1.21275
H,0,-3.6576,0.13267,-0.83505
H,0,-0.28737,0.20605,1.23737
C,0,1.15555,-1.09934,-0.30618
H,0,1.34179,-1.62185,-1.24854
C,0,2.45973,-0.84147,0.4376
H,0,0.47042,-1.71728,0.2894
H,0,2.95937,-1.79046,0.66417
H,0,3.13384,-0.23064,-0.17116
H,0,2.28229,-0.31706,1.38315
H,0,-1.01301,2.27151,-0.94157

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.136468	E(Thermal)=	0.146182
E(QCISD(T))=	-258.209037	E(Empiric)=	-0.121680
DE(Plus)=	-0.016679	DE(2DF)=	-0.246250
E(Delta-G3)=	-0.349405	E(G3-Empiric)=	-0.121680
G3(0 K)=	-258.806583	G3 Energy=	-258.796869
G3 Enthalpy=	-258.795925	G3 Free Energy=	-258.842567

6c-20 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -259.076633713

Zero-point correction= 0.141340 (Hartree/Particle)
Thermal correction to Energy= 0.150853
Thermal correction to Enthalpy= 0.151797
Thermal correction to Gibbs Free Energy= 0.105841
Sum of electronic and zero-point Energies= -258.935294
Sum of electronic and thermal Energies= -258.925781
Sum of electronic and thermal Enthalpies= -258.924837
Sum of electronic and thermal Free Energies= -258.970793

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.662	30.855	96.723

B3LYP/6-31+G*
E(RB3LYP) = -259.051502053

Zero-point correction= 0.142130 (Hartree/Particle)
Thermal correction to Energy= 0.150829
Thermal correction to Enthalpy= 0.151773
Thermal correction to Gibbs Free Energy= 0.108007
Sum of electronic and ZPE= -258.909372
Sum of electronic and thermal Energies= -258.900673
Sum of electronic and thermal Enthalpies= -258.899729
Sum of electronic and thermal Free Energies= -258.943495

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	94.647	28.785	92.114

C,0,0.32952,1.01508,0.61367
C,0,0.89683,1.48617,-0.50843
H,0,0.56314,1.22452,-1.50557
C,0,-1.28434,-0.36657,-0.46001
B,0,3.38267,-0.64507,-0.1404
H,0,0.67645,1.31876,1.59803
H,0,3.20944,-0.87562,1.01845
H,0,2.92205,-1.37249,-0.9684
H,0,4.08067,0.26651,-0.4695
H,0,1.70508,2.20321,-0.42488
C,0,-2.34719,-1.37541,-0.06272
H,0,-1.7131,0.46205,-1.04108
H,0,-0.49963,-0.83571,-1.06926
H,0,-2.82492,-1.78898,-0.95737
H,0,-1.90356,-2.1988,0.50561
H,0,-3.11784,-0.90446,0.55574
O,0,-0.69939,0.15151,0.73986

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.136445	E(Thermal)=	0.145351
E(QCISD(T))=	-258.210616	E(Empiric)=	-0.121680
DE(Plus)=	-0.016771	DE(2DF)=	-0.245862
E(Delta-G3)=	-0.349591	E(G3-Empiric)=	-0.121680

G3(0 K)=	-258.808075	G3 Energy=	-258.799168
G3 Enthalpy=	-258.798224	G3 Free Energy=	-258.842442

6d-1 Starting Material
B3LYP/6-31+G**
E(RB3LYP) = -271.764078014

Zero-point correction= 0.141365 (Hartree/Particle)
Thermal correction to Energy= 0.149140
Thermal correction to Enthalpy= 0.150084
Thermal correction to Gibbs Free Energy= 0.109141
Sum of electronic and ZPE= -271.622713
Sum of electronic and thermal Energies= -271.614938
Sum of electronic and thermal Enthalpies= -271.613994
Sum of electronic and thermal Free Energies= -271.654937

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	93.587	26.760	86.172

O,0,2.3162337546,0.6375450146,1.3254207802
C,0,2.4544729399,-0.5041091361,2.0666589269
C,0,1.8474463353,-0.9878908635,3.1677766593
C,0,0.7392614745,-0.3970191076,4.0099646697
C,0,1.3664922822,1.6407327633,1.6528010578
H,0,3.2407759018,-1.0940517714,1.6044550706
C,0,2.3203094147,-2.3355938527,3.6765791778
H,0,1.0775751569,-0.2842412758,5.0491665289
H,0,0.3724028462,0.5707949999,3.6768982607
H,0,-0.1170569169,-1.0847671886,4.0388977122
H,0,1.4870001818,2.4170715873,0.8947539443
H,0,0.3413048911,1.254310903,1.610364301
H,0,1.5607759637,2.0722116855,2.6418468711
H,0,2.6934214374,-2.258474802,4.7071754744
H,0,1.4954790725,-3.0612932805,3.6940206681
H,0,3.1217532642,-2.7552926753,3.0615248971

B3LYP/6-31G*
E(RB3LYP) = -271.739930847

Zero-point correction= 0.142556 (Hartree/Particle)
Thermal correction to Energy= 0.150226

Thermal correction to Enthalpy= 0.151170
Thermal correction to Gibbs Free Energy= 0.110741
Sum of electronic and ZPE= -271.597375
Sum of electronic and thermal Energies= -271.589705
Sum of electronic and thermal Enthalpies= -271.588761
Sum of electronic and thermal Free Energies= -271.629190

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.268	26.474	85.089

O,0,2.3188420693,0.6353794983,1.3240712154
C,0,2.4519107295,-0.5014360162,2.0675709525
C,0,1.8462858526,-0.9849661387,3.1668636335
C,0,0.7387562738,-0.3958058492,4.0096279177
C,0,1.3707294698,1.6339826387,1.6531257395
H,0,3.2386038851,-1.0933541027,1.6064461437
C,0,2.3202232057,-2.3316861686,3.6735792788
H,0,1.0753523799,-0.2828199552,5.0503953385
H,0,0.3704839162,0.5729538775,3.6775141448
H,0,-0.1190536314,-1.0831783841,4.0402988627
H,0,1.4871005208,2.4142411403,0.8968689653
H,0,0.3436704351,1.2497879001,1.6132582284
H,0,1.5614447913,2.0665843348,2.6433438957
H,0,2.6942113838,-2.2581695036,4.7052481555
H,0,1.4968489531,-3.0605964641,3.6925203092
H,0,3.1222377653,-2.7509838072,3.057572219

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.136854	E(Thermal)=	0.144728
E(QCISD(T))=	-270.893825	E(Empiric)=	-0.121680
DE(Plus)=	-0.016764	DE(2DF)=	-0.247348
E(Delta-G3)=	-0.356849	E(G3-Empiric)=	-0.121680
G3(0 K)=	-271.499612	G3 Energy=	-271.491737
G3 Enthalpy=	-271.490793	G3 Free Energy=	-271.531628

For Anharmonic Corrections of 6d-1

Zero-point vibrational energy 374281.6 (Joules/Mol)
89.45545 (Kcal/Mol)
Warning -- explicit consideration of 9 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 56.79 196.89 298.19 382.57 448.00
(Kelvin) 463.34 472.66 562.04 661.86 921.22

1198.32 1286.01 1383.29 1415.40 1490.79
1562.61 1602.07 1700.62 1716.43 1798.00
1837.44 2070.03 2079.25 2102.91 2160.74
2161.46 2182.52 2190.09 2202.20 2206.48
2221.56 2515.68 4339.16 4351.24 4360.15
4396.98 4399.69 4451.10 4485.03 4518.88
4590.31 4591.35

Zero-point correction= 0.142556 (Hartree/Particle)
Thermal correction to Energy= 0.150226
Thermal correction to Enthalpy= 0.151170
Thermal correction to Gibbs Free Energy= 0.110740
Sum of electronic and zero-point Energies= -271.597375
Sum of electronic and thermal Energies= -271.589705
Sum of electronic and thermal Enthalpies= -271.588760
Sum of electronic and thermal Free Energies= -271.629190

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.268	26.475	85.092

ZPE(harm) = 0.37428D+03 kJ/mol ZPE(anh)= 0.36776D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.21689D-63	0.71489D-63	
QZvib	0.80811D+02	0.19216D+02	
Energy	0.39442D+03	0.38628D+03	kJ/mol
Enthalpy	0.39690D+03	0.38876D+03	kJ/mol
Entropy	0.35602D+03	0.34695D+03	J/(mol K)
Sp.Heat(V)	0.11077D+03	0.10504D+03	J/(mol K)
Sp.Heat(P)	0.11908D+03	0.11336D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.21689D-63	0.71489D-63	
QZvib	0.80811D+02	0.19216D+02	
Energy	0.39442D+03	0.38628D+03	kJ/mol
Enthalpy	0.39690D+03	0.38876D+03	kJ/mol
Entropy	0.35602D+03	0.34695D+03	J/(mol K)
Sp.Heat(V)	0.11077D+03	0.10504D+03	J/(mol K)
Sp.Heat(P)	0.11908D+03	0.11336D+03	J/(mol K)

6d-2 Starting Material

B3LYP/6-31+G**

E(RB3LYP) = -271.772263383

Zero-point correction= 0.140478 (Hartree/Particle)

Thermal correction to Energy= 0.148514

Thermal correction to Enthalpy= 0.149458

Thermal correction to Gibbs Free Energy= 0.108343

Sum of electronic and zero-point Energies= -271.631785

Sum of electronic and thermal Energies= -271.623749

Sum of electronic and thermal Enthalpies= -271.622805

Sum of electronic and thermal Free Energies= -271.663920

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	93.194	27.182	86.535

Charge = 0 Multiplicity = 1

C,0,2.0353193624,0.4630575151,1.2328259695

C,0,2.4477136456,-0.7515573621,2.0219103742

C,0,1.8611915074,-1.0951630589,3.1774740001

O,0,0.8033683251,-0.4007819813,3.7115989157

H,0,1.2835737273,1.0517940537,1.7621726623

C,0,3.5478047932,-1.6061724037,1.4455417694

H,0,1.6194407573,0.174130274,0.2576737459

H,0,2.9022511944,1.1051774967,1.0269380629

H,0,2.1661154167,-1.9784379394,3.7401699908

C,0,0.6368822089,-0.5517898703,5.1156929873

H,0,-0.2846950697,-0.0304736207,5.3805967789

H,0,0.5433072951,-1.6114283859,5.3922961332

H,0,1.4774935574,-0.1086896511,5.6663996416

H,0,4.4656848389,-1.0210583326,1.2986982043

H,0,3.7893686236,-2.4561734479,2.0919430609

H,0,3.2671078165,-2.0037102857,0.460477703

B3LYP/6-31G*

E(RB3LYP) = -271.747595364

Zero-point correction= 0.141627 (Hartree/Particle)

Thermal correction to Energy= 0.149592

Thermal correction to Enthalpy= 0.150536

Thermal correction to Gibbs Free Energy= 0.109648

Sum of electronic and zero-point Energies= -271.605968

Sum of electronic and thermal Energies= -271.598003

Sum of electronic and thermal Enthalpies= -271.597059

Sum of electronic and thermal Free Energies= -271.637947

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.870	26.931	86.057

C,0,2.0357574206,0.4650154926,1.243539837
C,0,2.4413334862,-0.7589010509,2.021310443
C,0,1.8469678676,-1.110495261,3.1679158961
O,0,0.7842617622,-0.424928046,3.6976733
H,0,1.283228846,1.0483257745,1.7789078625
C,0,3.544989852,-1.6093286694,1.4485788711
H,0,1.6220588925,0.1919491594,0.2621566029
H,0,2.9040481819,1.1099726555,1.0480059334
H,0,2.1502137056,-1.9974651748,3.7277478803
C,0,0.6456834265,-0.5427035048,5.1040389919
H,0,-0.2874793806,-0.0419707932,5.3718450624
H,0,0.5884140975,-1.5966646294,5.4144820415
H,0,1.4795018818,-0.0625533109,5.6352257628
H,0,4.4668581751,-1.0256858305,1.3138632506
H,0,3.7800183427,-2.4655416888,2.0905052445
H,0,3.2760714423,-2.0003021223,0.45661302

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.135962	E(Thermal)=	0.144128
E(QCISD(T))=	-270.901979	E(Empiric)=	-0.121680
DE(Plus)=	-0.017435	DE(2DF)=	-0.246476
E(Delta-G3)=	-0.356150	E(G3-Empiric)=	-0.121680
G3(0 K)=	-271.507758	G3 Energy=	-271.499592
G3 Enthalpy=	-271.498647	G3 Free Energy=	-271.539951

For Anharmonic Corrections of 6d-2

Zero-point vibrational energy 371841.4 (Joules/Mol)
88.87224 (Kcal/Mol)
Warning -- explicit consideration of 10 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 88.02 212.35 232.98 271.85 303.33
(Kelvin) 432.73 483.19 585.42 683.62 795.41
1217.06 1244.37 1414.44 1466.63 1478.28
1576.21 1607.05 1702.99 1708.29 1797.55
1834.57 2013.55 2068.21 2088.16 2160.65
2162.49 2181.96 2184.62 2191.98 2201.85
2209.52 2545.97 4332.05 4343.30 4354.53
4404.13 4409.69 4410.48 4474.02 4510.08
4529.70 4531.11

Zero-point correction= 0.141627 (Hartree/Particle)
Thermal correction to Energy= 0.149592
Thermal correction to Enthalpy= 0.150536
Thermal correction to Gibbs Free Energy= 0.109647
Sum of electronic and zero-point Energies= -271.605968
Sum of electronic and thermal Energies= -271.598003
Sum of electronic and thermal Enthalpies= -271.597059
Sum of electronic and thermal Free Energies= -271.637948

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.870	26.931	86.058

ZPE(harm) = 0.37184D+03 kJ/mol ZPE(anh)= 0.36638D+03 kJ/mol
Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.65578D-63	0.86765D-62	
QZvib	0.91302D+02	0.13319D+03	
Energy	0.39275D+03	0.38743D+03	kJ/mol
Enthalpy	0.39523D+03	0.38990D+03	kJ/mol
Entropy	0.36007D+03	0.36367D+03	J/(mol K)
Sp.Heat(V)	0.11268D+03	0.11410D+03	J/(mol K)
Sp.Heat(P)	0.12099D+03	0.12242D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.65578D-63	0.86765D-62	
QZvib	0.91302D+02	0.13319D+03	
Energy	0.39275D+03	0.38743D+03	kJ/mol
Enthalpy	0.39523D+03	0.38990D+03	kJ/mol
Entropy	0.36007D+03	0.36367D+03	J/(mol K)
Sp.Heat(V)	0.11268D+03	0.11410D+03	J/(mol K)
Sp.Heat(P)	0.12099D+03	0.12242D+03	J/(mol K)

6d-3 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -298.390911998

Zero-point correction= 0.172347 (Hartree/Particle)
Thermal correction to Energy= 0.181381
Thermal correction to Enthalpy= 0.182325
Thermal correction to Gibbs Free Energy= 0.139520

Sum of electronic and ZPE= -298.218565
Sum of electronic and thermal Energies= -298.209531
Sum of electronic and thermal Enthalpies= -298.208587
Sum of electronic and thermal Free Energies= -298.251392

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.818	33.191	90.091

C,0,0.9266691744,-0.1159689038,4.2976409052
C,0,2.0210929723,-0.801485956,3.4919023347
B,0,3.5967621838,-0.0933148495,3.7267259676
C,0,2.4873243862,-0.2054323562,2.2900990674
O,0,2.005747243,1.0072277281,1.8212892764
C,0,0.9159448582,0.8378511025,0.9116770681
C,0,2.031938174,-2.3209468102,3.5940098151
H,0,2.9224272074,-0.8467975249,1.5194544186
H,0,3.941360474,0.4621873299,2.6710123811
H,0,3.4559021073,0.8200151896,4.4832450591
H,0,4.4062792744,-0.9619870626,3.8670532331
H,0,1.0577385858,-0.3149367526,5.3658274431
H,0,0.9342178118,0.9653154848,4.1504090038
H,0,-0.0605214899,-0.5020141455,4.0083090668
H,0,0.6313907935,1.8399503551,0.5878643011
H,0,1.220439358,0.247243384,0.0364018767
H,0,0.0603813513,0.3523672515,1.3972393514
H,0,2.2394490091,-2.638741347,4.6209556217
H,0,1.054964226,-2.7331235834,3.3067869691
H,0,2.7957732994,-2.7680515338,2.9512688399

B3LYP/6-31G*
E(RB3LYP) = -298.363637702

Zero-point correction= 0.173651 (Hartree/Particle)
Thermal correction to Energy= 0.182628
Thermal correction to Enthalpy= 0.183572
Thermal correction to Gibbs Free Energy= 0.140858
Sum of electronic and ZPE= -298.189987
Sum of electronic and thermal Energies= -298.181009
Sum of electronic and thermal Enthalpies= -298.180065
Sum of electronic and thermal Free Energies= -298.222779

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	114.601	32.868	89.900

C,0,0.9274413757,-0.1150238561,4.2934412613
C,0,2.0296877613,-0.8007251031,3.498404827
B,0,3.5893961669,-0.0964532869,3.7376733974
C,0,2.4896148763,-0.202772921,2.2906182543
O,0,2.0068244312,1.0090165167,1.8271312661
C,0,0.9190654418,0.8371419159,0.9210975423
C,0,2.0335124716,-2.3206031697,3.5913052932
H,0,2.9140427892,-0.8473159112,1.5152777641
H,0,3.9292319607,0.439676988,2.6622249618
H,0,3.4631867511,0.8367931991,4.4737118515
H,0,4.4100443969,-0.9565116842,3.8750619458
H,0,1.0513979831,-0.3051339647,5.3646837725
H,0,0.9332526157,0.9655949825,4.1376685224
H,0,-0.0587666917,-0.5042012021,4.0020916176
H,0,0.6308923923,1.8391683403,0.5978683377
H,0,1.2211372749,0.2474105087,0.0432137217
H,0,0.0629482528,0.3481899809,1.4035923873
H,0,2.2363893211,-2.6464208988,4.6172986442
H,0,1.0569412752,-2.7315022527,3.2982078974
H,0,2.799040154,-2.7669711817,2.9485987344

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.167220	E(Thermal)=	0.177368
E(QCISD(T))=	-297.410866	E(Empiric)=	-0.141960
DE(Plus)=	-0.018154	DE(2DF)=	-0.288793
E(Delta-G3)=	-0.404752	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.097305	G3 Energy=	-298.087157
G3 Enthalpy=	-298.086213	G3 Free Energy=	-298.130918

For Anharmonic Corrections of 6d-3

Zero-point vibrational energy 456029.5 (Joules/Mol)
108.99367 (Kcal/Mol)
Warning -- explicit consideration of 12 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 99.73 216.75 262.56 313.94 347.91
(Kelvin) 364.90 432.27 488.97 508.84 558.98
654.50 826.79 961.90 1111.07 1172.83
1219.05 1415.13 1430.75 1490.86 1535.62
1539.27 1615.34 1630.83 1671.85 1688.27

1706.88 1733.96 1782.54 1813.56 1972.58
2062.88 2085.72 2126.11 2172.28 2177.80
2184.45 2192.14 2203.54 2208.93 2243.19
3398.98 3710.23 3859.50 4347.28 4360.45
4367.25 4436.13 4459.64 4465.95 4471.31
4501.34 4543.00 4548.83

Zero-point correction= 0.173692 (Hartree/Particle)
Thermal correction to Energy= 0.182687
Thermal correction to Enthalpy= 0.183631
Thermal correction to Gibbs Free Energy= 0.140893
Sum of electronic and zero-point Energies= -298.189986
Sum of electronic and thermal Energies= -298.180991
Sum of electronic and thermal Enthalpies= -298.180047
Sum of electronic and thermal Free Energies= -298.222786

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	114.638	32.931	89.950

ZPE(harm) = 0.45603D+03 kJ/mol ZPE(anh)= 0.44817D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.15683D-77	0.12708D-75	
QZvib	0.12253D+03	0.41764D+03	
Energy	0.47965D+03	0.47298D+03	kJ/mol
Enthalpy	0.48212D+03	0.47545D+03	kJ/mol
Entropy	0.38467D+03	0.39884D+03	J/(mol K)
Sp.Heat(V)	0.13778D+03	0.14143D+03	J/(mol K)
Sp.Heat(P)	0.14610D+03	0.14975D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.15683D-77	0.12708D-75	
QZvib	0.12253D+03	0.41764D+03	
Energy	0.47965D+03	0.47298D+03	kJ/mol
Enthalpy	0.48212D+03	0.47545D+03	kJ/mol
Entropy	0.38467D+03	0.39884D+03	J/(mol K)
Sp.Heat(V)	0.13778D+03	0.14143D+03	J/(mol K)
Sp.Heat(P)	0.14610D+03	0.14975D+03	J/(mol K)

6d-4 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -298.400413659

Zero-point correction= 0.172510 (Hartree/Particle)
Thermal correction to Energy= 0.181388
Thermal correction to Enthalpy= 0.182333
Thermal correction to Gibbs Free Energy= 0.140127
Sum of electronic and ZPE= -298.227904
Sum of electronic and thermal Energies= -298.219025
Sum of electronic and thermal Enthalpies= -298.218081
Sum of electronic and thermal Free Energies= -298.260287

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.823	32.941	88.829

C,0,1.9591345865,0.4758625775,1.2281089111
C,0,2.7239826008,-0.5500983812,2.0581201447
C,0,2.1293569294,-0.9981728388,3.2848331833
O,0,0.9437286508,-0.481675356,3.6954615093
H,0,1.4552129839,1.2139387644,1.8541336945
B,0,3.6588457587,0.0977322662,3.3122395956
C,0,3.4355445097,-1.6125407054,1.223624924
H,0,1.2025435146,-0.0149971902,0.6013210524
H,0,2.650993069,1.0069000372,0.5663852779
H,0,4.7389576789,-0.4180160686,3.3780245188
H,0,3.4822258013,1.2790793518,3.3965341731
H,0,3.1147061046,-0.3320912247,4.373738771
H,0,2.3588900415,-2.000260635,3.6533788181
C,0,0.6085703145,-0.7259912517,5.0631731656
H,0,-0.3943340328,-0.3256690224,5.2122756772
H,0,0.6141292993,-1.8011600516,5.2823965607
H,0,1.3178385277,-0.2110555123,5.7234095142
H,0,4.2095364246,-1.1495219502,0.6026488518
H,0,3.9280865178,-2.3626911751,1.8501909707
H,0,2.7330147193,-2.1293036338,0.5555656858

B3LYP/6-31G*
E(RB3LYP) = -298.373105511

Zero-point correction= 0.173840 (Hartree/Particle)
Thermal correction to Energy= 0.182662
Thermal correction to Enthalpy= 0.183607

Thermal correction to Gibbs Free Energy= 0.141496
Sum of electronic and ZPE= -298.199266
Sum of electronic and thermal Energies= -298.190443
Sum of electronic and thermal Enthalpies= -298.189499
Sum of electronic and thermal Free Energies= -298.231610

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	114.622	32.621	88.630

C,0,1.956595774,0.4734051801,1.233589887
C,0,2.7320353675,-0.5471189326,2.0604208129
C,0,2.1340443188,-0.9978967532,3.2894148162
O,0,0.9458001801,-0.4835105696,3.690383294
H,0,1.4538604872,1.2102022665,1.8630810913
B,0,3.6620594968,0.1008207962,3.3051231035
C,0,3.4370401378,-1.611164531,1.2233977924
H,0,1.1967331104,-0.0192961408,0.6111385346
H,0,2.6405776873,1.0081492688,0.5657136308
H,0,4.740791016,-0.4171789913,3.3873595291
H,0,3.4828621241,1.2809510362,3.407611723
H,0,3.1050016552,-0.344142555,4.3640760216
H,0,2.3594294008,-2.0035981828,3.6532333152
C,0,0.6100536425,-0.7222304494,5.0550270781
H,0,-0.3917242605,-0.3170359045,5.2039155203
H,0,0.610772489,-1.796994182,5.2809183959
H,0,1.3210844778,-0.2105751331,5.7172230322
H,0,4.2098988359,-1.150718384,0.5980629345
H,0,3.9313044136,-2.362431217,1.848605576
H,0,2.7327436455,-2.1293686214,0.5572689114

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.166886	E(Thermal)=	0.175987
E(QCISD(T))=	-297.404001	E(Empiric)=	-0.141960
DE(Plus)=	-0.018363	DE(2DF)=	-0.290156
E(Delta-G3)=	-0.403489	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.091083	G3 Energy=	-298.081982
G3 Enthalpy=	-298.081038	G3 Free Energy=	-298.123677

For Anharmonic Corrections of 6d-4

Zero-point vibrational energy 456418.0 (Joules/Mol)
109.08652 (Kcal/Mol)
Warning -- explicit consideration of 12 degrees of freedom as

vibrations may cause significant error
Vibrational temperatures: 176.11 232.97 256.98 314.03 348.15
(Kelvin) 353.67 444.86 472.99 513.85 571.72
728.83 790.59 1021.83 1107.91 1188.37
1244.75 1419.30 1438.35 1497.55 1525.10
1542.09 1628.81 1641.00 1691.03 1706.33
1712.95 1751.04 1831.43 1853.91 1962.07
2064.79 2085.76 2120.22 2175.10 2178.78
2183.78 2193.21 2196.93 2204.90 2236.15
3139.43 3681.66 3828.92 4358.32 4359.74
4371.30 4447.22 4455.39 4464.61 4480.46
4491.46 4539.54 4562.55

Zero-point correction= 0.173840 (Hartree/Particle)
Thermal correction to Energy= 0.182663
Thermal correction to Enthalpy= 0.183607
Thermal correction to Gibbs Free Energy= 0.141496
Sum of electronic and zero-point Energies= -298.199265
Sum of electronic and thermal Energies= -298.190443
Sum of electronic and thermal Enthalpies= -298.189498
Sum of electronic and thermal Free Energies= -298.231610

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	114.623	32.621	88.630

ZPE(harm) = 0.45642D+03 kJ/mol ZPE(anh)= 0.44882D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.80487D-78	0.30125D-76	
QZvib	0.73553D+02	0.12858D+03	
Energy	0.47958D+03	0.47289D+03	kJ/mol
Enthalpy	0.48206D+03	0.47537D+03	kJ/mol
Entropy	0.37914D+03	0.38682D+03	J/(mol K)
Sp.Heat(V)	0.13649D+03	0.13989D+03	J/(mol K)
Sp.Heat(P)	0.14480D+03	0.14820D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.80487D-78	0.30125D-76	
QZvib	0.73553D+02	0.12858D+03	
Energy	0.47958D+03	0.47289D+03	kJ/mol
Enthalpy	0.48206D+03	0.47537D+03	kJ/mol
Entropy	0.37914D+03	0.38682D+03	J/(mol K)

Sp.Heat(V)	0.13649D+03	0.13989D+03	J/(mol K)
Sp.Heat(P)	0.14480D+03	0.14820D+03	J/(mol K)

6d-5 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -298.395179068

Zero-point correction= 0.172028 (Hartree/Particle)
Thermal correction to Energy= 0.181025
Thermal correction to Enthalpy= 0.181969
Thermal correction to Gibbs Free Energy= 0.139404
Sum of electronic and ZPE= -298.223151
Sum of electronic and thermal Energies= -298.214154
Sum of electronic and thermal Enthalpies= -298.213210
Sum of electronic and thermal Free Energies= -298.255775

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.595	33.374	89.586

C,0,0.8188956441,-0.8482050958,4.5536576642
C,0,1.9174424961,-0.8925977621,3.514904242
C,0,2.5249033177,-2.2467022253,3.2213774722
B,0,3.256618488,0.4327812619,3.6759214805
C,0,2.0075904624,0.1290912214,2.5325006994
O,0,1.0507920415,1.1510417837,2.4802485008
C,0,0.031263137,0.8998651184,1.5199531469
H,0,2.4401718533,-0.1187835452,1.5622837775
H,0,4.3153913803,0.195203349,3.1679737784
H,0,2.9639529706,1.4870760016,4.1591738936
H,0,3.1514280429,-0.3627523247,4.6147204036
H,0,1.1108491087,-1.3800217341,5.4637050687
H,0,0.5519682877,0.1791465416,4.8034268356
H,0,-0.0704275666,-1.3425914028,4.1425898553
H,0,-0.6319845759,1.7673650567,1.5320703564
H,0,0.4537294063,0.7853883222,0.5108438195
H,0,-0.5476589579,-0.002512486,1.7651366294
H,0,2.8786638812,-2.735637384,4.1341536235
H,0,1.754214839,-2.8828360878,2.7681885014
H,0,3.3605477435,-2.1700206087,2.5218202512

B3LYP/6-31G*
E(RB3LYP) = -298.367498307

Zero-point correction= 0.173354 (Hartree/Particle)
Thermal correction to Energy= 0.182241
Thermal correction to Enthalpy= 0.183185
Thermal correction to Gibbs Free Energy= 0.140906
Sum of electronic and ZPE= -298.194144
Sum of electronic and thermal Energies= -298.185257
Sum of electronic and thermal Enthalpies= -298.184313
Sum of electronic and thermal Free Energies= -298.226592

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	114.358	33.001	88.984

C,0,0.814337135,-0.8349891525,4.5372078972
C,0,1.9266920372,-0.8844480013,3.5128579535
C,0,2.5232662419,-2.2425388966,3.2149974681
B,0,3.2598380859,0.4401112638,3.6698301933
C,0,2.0261653919,0.1424589678,2.5299969325
O,0,1.0659670741,1.1600685013,2.4754973949
C,0,0.0326063993,0.8820857758,1.5439298709
H,0,2.4470740105,-0.1180828774,1.5568208058
H,0,4.3272962184,0.1919421814,3.1841178125
H,0,2.9753485823,1.4840943032,4.1816936548
H,0,3.1359027652,-0.373318339,4.600328244
H,0,1.0910339713,-1.360553914,5.4563842057
H,0,0.5449856487,0.1951078207,4.7742140852
H,0,-0.0701902264,-1.3317918658,4.1171691326
H,0,-0.6361618854,1.7465542545,1.548055108
H,0,0.4322137511,0.7448938337,0.5271718572
H,0,-0.5404773001,-0.0175255909,1.8159175581
H,0,2.8572217728,-2.7473417604,4.1273452801
H,0,1.7538480967,-2.8663495861,2.7415874107
H,0,3.3713842296,-2.1660789181,2.5295271351

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.166420	E(Thermal)=	0.175590
E(QCISD(T))=	-297.398396	E(Empiric)=	-0.141960
DE(Plus)=	-0.019258	DE(2DF)=	-0.289360
E(Delta-G3)=	-0.403456	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.086010	G3 Energy=	-298.076840
G3 Enthalpy=	-298.075896	G3 Free Energy=	-298.118711

For Anharmonic Corrections of 6d-5

Zero-point vibrational energy 455144.5 (Joules/Mol)
108.78215 (Kcal/Mol)
Warning -- explicit consideration of 13 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 144.72 230.71 262.33 308.21 336.29
(Kelvin) 379.10 408.64 489.33 575.94 607.10
722.41 824.75 853.34 1100.22 1156.94
1210.74 1391.01 1410.70 1458.51 1510.70
1538.00 1568.27 1642.98 1647.81 1679.91
1688.85 1709.56 1779.69 1819.23 1966.65
2064.09 2082.63 2113.44 2167.07 2169.49
2176.20 2181.82 2202.60 2209.42 2223.29
3393.06 3687.98 3840.98 4315.08 4383.48
4386.38 4393.60 4480.85 4485.37 4486.56
4519.63 4529.10 4567.68

Zero-point correction= 0.173355 (Hartree/Particle)
Thermal correction to Energy= 0.182242
Thermal correction to Enthalpy= 0.183186
Thermal correction to Gibbs Free Energy= 0.140907
Sum of electronic and zero-point Energies= -298.194143
Sum of electronic and thermal Energies= -298.185256
Sum of electronic and thermal Enthalpies= -298.184312
Sum of electronic and thermal Free Energies= -298.226591

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	114.359	33.001	88.984

ZPE(harm) = 0.45514D+03 kJ/mol ZPE(anh)= 0.44786D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.15346D-77	0.75300D-76	
QZvib	0.83902D+02	0.21804D+03	
Energy	0.47848D+03	0.47234D+03	kJ/mol
Enthalpy	0.48096D+03	0.47481D+03	kJ/mol
Entropy	0.38062D+03	0.39240D+03	J/(mol K)
Sp.Heat(V)	0.13808D+03	0.14124D+03	J/(mol K)
Sp.Heat(P)	0.14639D+03	0.14956D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.15346D-77	0.75300D-76	
QZvib	0.83902D+02	0.21804D+03	
Energy	0.47848D+03	0.47234D+03	kJ/mol
Enthalpy	0.48096D+03	0.47481D+03	kJ/mol
Entropy	0.38062D+03	0.39240D+03	J/(mol K)
Sp.Heat(V)	0.13808D+03	0.14124D+03	J/(mol K)
Sp.Heat(P)	0.14639D+03	0.14956D+03	J/(mol K)

6d-6 Transition State

B3LYP/6-31+G**

E(RB3LYP) = -298.400109668

Zero-point correction= 0.172458 (Hartree/Particle)
Thermal correction to Energy= 0.181292
Thermal correction to Enthalpy= 0.182236
Thermal correction to Gibbs Free Energy= 0.140174
Sum of electronic and ZPE= -298.227651
Sum of electronic and thermal Energies= -298.218818
Sum of electronic and thermal Enthalpies= -298.217874
Sum of electronic and thermal Free Energies= -298.259936

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	113.762	33.091	88.528

C,0,2.1183846931,0.5191804963,1.3252572553
C,0,2.7425559131,-0.5951973629,2.1368054142
C,0,2.1138010416,-1.0181946487,3.3425232524
O,0,0.8705800267,-0.4590078061,3.6490741797
H,0,1.6934160365,1.2895655831,1.9689597265
B,0,3.5102546426,-0.1282936798,3.7772357513
C,0,3.5793790571,-1.6010776571,1.3737795904
H,0,1.3012340359,0.0953840367,0.7291670903
H,0,2.8478986496,0.9694789459,0.6455715586
H,0,3.9957877283,0.316913575,2.7207529449
H,0,3.1343332134,0.8651397536,4.3308138317
H,0,4.3546272839,-0.8565506082,4.2141595486
H,0,2.2051078975,-2.0683621336,3.6258596725
C,0,0.5466580984,-0.5094494611,5.0323466518
H,0,-0.4534864681,-0.0836232732,5.1353014475

H,0,0.5365001796,-1.5462669712,5.399127007
H,0,1.2620849354,0.0739749264,5.6253349059
H,0,4.3644916079,-1.1087659314,0.7914987754
H,0,4.046290271,-2.3263276991,2.0444651068
H,0,2.9265391564,-2.1447580849,0.6801692891

B3LYP/6-31G*
E(RB3LYP) = -298.372002091

Zero-point correction= 0.173723 (Hartree/Particle)
Thermal correction to Energy= 0.182491
Thermal correction to Enthalpy= 0.183435
Thermal correction to Gibbs Free Energy= 0.141483
Sum of electronic and ZPE= -298.198279
Sum of electronic and thermal Energies= -298.189511
Sum of electronic and thermal Enthalpies= -298.188567
Sum of electronic and thermal Free Energies= -298.230519

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	114.515	32.752	88.297

C,0,2.1151776597,0.5185580732,1.335195849
C,0,2.7499973507,-0.594750321,2.1410012793
C,0,2.1180639414,-1.0237605315,3.3478350495
O,0,0.8701448499,-0.4694504568,3.6400992234
H,0,1.6848570188,1.2807902187,1.9856733275
B,0,3.5027722707,-0.1417307744,3.7889466335
C,0,3.5834371761,-1.5984058799,1.371263148
H,0,1.2998984684,0.0909417911,0.7383544222
H,0,2.837533746,0.9808056922,0.6548141231
H,0,3.9820522282,0.3040311465,2.7211713885
H,0,3.1401369369,0.8615195146,4.3356093103
H,0,4.3611083338,-0.8629976601,4.2117289023
H,0,2.2046588041,-2.0789219224,3.6177729982
C,0,0.5491155712,-0.4992739715,5.0201485544
H,0,-0.4522697242,-0.0725379652,5.1187347142
H,0,0.5386126672,-1.5298163012,5.407472436
H,0,1.2628724575,0.0919895415,5.6087546499
H,0,4.3636490726,-1.1056385721,0.7816484932
H,0,4.0572133784,-2.3223193746,2.0396768284
H,0,2.9274057927,-2.1452702471,0.6823016692

Temperature= 298.150000 Pressure= 1.000000

E(ZPE)=	0.168794	E(Thermal)=	0.178606
E(QCISD(T))=	-297.424582	E(Empiric)=	-0.141960
DE(Plus)=	-0.018255	DE(2DF)=	-0.288112
E(Delta-G3)=	-0.403948	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.108064	G3 Energy=	-298.098252
G3 Enthalpy=	-298.097308	G3 Free Energy=	-298.141798

For Anharmonic Correction Of 6d-6

Zero-point vibrational energy 456111.1 (Joules/Mol)
109.01317 (Kcal/Mol)
Warning -- explicit consideration of 13 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 174.43 248.84 261.64 306.83 331.45
(Kelvin) 354.12 469.96 481.81 541.22 669.40
753.05 837.93 861.75 1065.40 1183.03
1221.27 1392.89 1423.17 1467.70 1510.24
1548.01 1580.43 1648.80 1656.53 1702.93
1707.39 1717.03 1775.96 1835.35 1953.86
2063.39 2083.51 2117.20 2163.39 2169.25
2172.40 2180.76 2199.49 2210.96 2225.81
3327.32 3685.42 3831.82 4329.94 4390.41
4400.40 4422.42 4469.73 4483.35 4489.69
4520.86 4526.29 4568.73

Zero-point correction= 0.173724 (Hartree/Particle)
Thermal correction to Energy= 0.182492
Thermal correction to Enthalpy= 0.183436
Thermal correction to Gibbs Free Energy= 0.141483
Sum of electronic and zero-point Energies= -298.198279
Sum of electronic and thermal Energies= -298.189510
Sum of electronic and thermal Enthalpies= -298.188566
Sum of electronic and thermal Free Energies= -298.230519

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	114.515	32.752	88.297

ZPE(harm) = 0.45611D+03 kJ/mol ZPE(anh)= 0.44889D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.83321D-78	0.19306D-76	
QZvib	0.67277D+02	0.84504D+02	
Energy	0.47913D+03	0.47240D+03	kJ/mol

Enthalpy	0.48161D+03	0.47487D+03	kJ/mol
Entropy	0.37775D+03	0.38129D+03	J/(mol K)
Sp.Heat(V)	0.13703D+03	0.13980D+03	J/(mol K)
Sp.Heat(P)	0.14535D+03	0.14812D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.83321D-78	0.19306D-76	
QZvib	0.67277D+02	0.84504D+02	
Energy	0.47913D+03	0.47240D+03	kJ/mol
Enthalpy	0.48161D+03	0.47487D+03	kJ/mol
Entropy	0.37775D+03	0.38129D+03	J/(mol K)
Sp.Heat(V)	0.13703D+03	0.13980D+03	J/(mol K)
Sp.Heat(P)	0.14535D+03	0.14812D+03	J/(mol K)

6d-7 Complex
B3LYP/6-31+G**
E(RB3LYP) = -298.421817199

Zero-point correction= 0.174353 (Hartree/Particle)
Thermal correction to Energy= 0.184130
Thermal correction to Enthalpy= 0.185074
Thermal correction to Gibbs Free Energy= 0.140081
Sum of electronic and ZPE= -298.247464
Sum of electronic and thermal Energies= -298.237687
Sum of electronic and thermal Enthalpies= -298.236743
Sum of electronic and thermal Free Energies= -298.281736

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	115.543	34.654	94.696

C,0,1.6227416426,-0.0158324932,1.0074608148
C,0,2.7923781086,-0.2365514752,1.9799416511
C,0,2.267948867,-0.7120415174,3.3707406928
O,0,1.317112905,0.2747446122,3.8142797392
H,0,0.8862829891,0.6742493158,1.4236438771
B,0,3.4144506621,-0.9956763883,4.4083731053
C,0,3.8174816579,-1.2103908302,1.3756358586
H,0,1.1181372013,-0.9664249502,0.7900035588
H,0,1.9880908156,0.3937182527,0.0587832483
H,0,3.2839578501,0.7335143033,2.1383488139

H,0,3.5211955249,-0.3421336006,5.4030121187
H,0,4.1979935969,-1.8760001722,4.2151083652
H,0,1.7248583223,-1.6639241286,3.183393708
C,0,0.4957766511,-0.1634667378,4.876365434
H,0,-0.1792675296,0.659564437,5.1236358576
H,0,-0.1025669784,-1.0424153221,4.5850820695
H,0,1.0802323838,-0.4204441157,5.7738025675
H,0,4.0873680723,-0.888076929,0.3643205706
H,0,4.7388289655,-1.2736120543,1.961351982
H,0,3.4025082917,-2.2231192061,1.2982639671

B3LYP/6-31G*
E(RB3LYP) = -298.394506350

Zero-point correction= 0.175684 (Hartree/Particle)
Thermal correction to Energy= 0.185417
Thermal correction to Enthalpy= 0.186361
Thermal correction to Gibbs Free Energy= 0.141511
Sum of electronic and ZPE= -298.218822
Sum of electronic and thermal Energies= -298.209090
Sum of electronic and thermal Enthalpies= -298.208146
Sum of electronic and thermal Free Energies= -298.252995

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	116.351	34.405	94.394

C,0,1.621333841,-0.0124081924,1.0140255024
C,0,2.7910704052,-0.2402551928,1.9833719946
C,0,2.2597891044,-0.7204594883,3.3709042295
O,0,1.31682282,0.2701674489,3.8120689537
H,0,0.8833155716,0.6684558917,1.4430219694
B,0,3.4190364141,-0.9833416089,4.4011943235
C,0,3.8143828599,-1.2133476299,1.3775649599
H,0,1.1196017268,-0.9622091643,0.7849803412
H,0,1.9828810104,0.411338915,0.0694706358
H,0,3.2840163263,0.7284173939,2.147577796
H,0,3.5706659054,-0.271744603,5.350654441
H,0,4.174958184,-1.8964732309,4.2453750952
H,0,1.7176658165,-1.6711371029,3.1814059785
C,0,0.4982455801,-0.1716237897,4.869106778
H,0,-0.1739330481,0.652201865,5.1254103528
H,0,-0.1064126805,-1.047965352,4.5791028292
H,0,1.0813759195,-0.4392428193,5.7662001028

H,0,4.0926907654,-0.8859203991,0.3694394093
H,0,4.7324928074,-1.2845986573,1.9692362732
H,0,3.3955106706,-2.2241732837,1.291436034

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.168657	E(Thermal)=	0.178665
E(QCISD(T))=	-297.426531	E(Empiric)=	-0.141960
DE(Plus)=	-0.018405	DE(2DF)=	-0.287478
E(Delta-G3)=	-0.403787	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.109504	G3 Energy=	-298.099496
G3 Enthalpy=	-298.098552	G3 Free Energy=	-298.143963

6d-8 Complex
B3LYP/6-31+G**
E(RB3LYP) = -298.406961848

Zero-point correction= 0.172794 (Hartree/Particle)
Thermal correction to Energy= 0.182743
Thermal correction to Enthalpy= 0.183687
Thermal correction to Gibbs Free Energy= 0.139329
Sum of electronic and ZPE= -298.234168
Sum of electronic and thermal Energies= -298.224219
Sum of electronic and thermal Enthalpies= -298.223275
Sum of electronic and thermal Free Energies= -298.267633

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	114.673	35.921	93.360

C,0,2.1260545127,0.4995967516,1.3067192591
C,0,2.6452775082,-0.6454126681,2.1460838433
C,0,1.9975697158,-1.0023773264,3.3027660539
O,0,0.8691108094,-0.3736876877,3.7064491152
H,0,1.6636778449,1.273169155,1.9217070268
B,0,3.7408021997,0.012616525,3.6924122577
C,0,3.5556759988,-1.6367833395,1.4555166095
H,0,1.3681012581,0.1265384403,0.6053745466
H,0,2.9366938168,0.9468334475,0.7249221471
H,0,4.2344515885,0.7652660318,2.8942150263
H,0,3.1461034604,0.6063352529,4.5536316058
H,0,4.4412819611,-0.8977835721,4.0418357655

H,0,2.2475253039,-1.9205718443,3.8326283702
C,0,0.5389952089,-0.5151237985,5.0918117479
H,0,-0.460974138,-0.0974398746,5.2116423857
H,0,0.5332125588,-1.572947653,5.3834934002
H,0,1.2545177897,0.0358037117,5.7105724584
H,0,4.4548991917,-1.1401885594,1.0790579655
H,0,3.8659625735,-2.4455757224,2.1213594218
H,0,3.0290578373,-2.0780842699,0.5992819939

B3LYP/6-31G*
E(RB3LYP) = -298.380589869

Zero-point correction= 0.174187 (Hartree/Particle)
Thermal correction to Energy= 0.184042
Thermal correction to Enthalpy= 0.184986
Thermal correction to Gibbs Free Energy= 0.140867
Sum of electronic and ZPE= -298.206402
Sum of electronic and thermal Energies= -298.196548
Sum of electronic and thermal Enthalpies= -298.195604
Sum of electronic and thermal Free Energies= -298.239723

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	115.488	35.606	92.856

C,0,2.1245584485,0.4970036188,1.3106323972
C,0,2.6450087623,-0.6490017435,2.1488861351
C,0,1.9918550914,-1.0060892668,3.3020465085
O,0,0.8650087513,-0.3780679166,3.7010303722
H,0,1.6518330519,1.2634315859,1.9276851886
B,0,3.7410497051,0.0100056931,3.6855010338
C,0,3.556063762,-1.639181041,1.4578011976
H,0,1.3750185695,0.1253572529,0.5986669862
H,0,2.9367008064,0.9551971503,0.7384942529
H,0,4.2187408386,0.7917583757,2.9039184686
H,0,3.1441840277,0.5753830975,4.5666844933
H,0,4.4535474272,-0.8995222574,4.0141294637
H,0,2.2454124152,-1.9207118301,3.8377177127
C,0,0.542445989,-0.5078786965,5.0859592977
H,0,-0.4583946962,-0.090843224,5.2076858881
H,0,0.5396982959,-1.5630773073,5.3899707696
H,0,1.2596582732,0.0482163653,5.6988104412
H,0,4.4601029811,-1.1435043093,1.0904152662
H,0,3.8597078758,-2.4531098102,2.1214889289

H,0,3.0357966243,-2.0751827369,0.5939561982

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.167220	E(Thermal)=	0.177368
E(QCISD(T))=	-297.410866	E(Empiric)=	-0.141960
DE(Plus)=	-0.018154	DE(2DF)=	-0.288794
E(Delta-G3)=	-0.404752	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.097306	G3 Energy=	-298.087158
G3 Enthalpy=	-298.086214	G3 Free Energy=	-298.130919

For Anharmonic Corrections of 6d-8

Zero-point correction= 0.174188 (Hartree/Particle)
Thermal correction to Energy= 0.184042
Thermal correction to Enthalpy= 0.184986
Thermal correction to Gibbs Free Energy= 0.140867
Sum of electronic and zero-point Energies= -298.206402
Sum of electronic and thermal Energies= -298.196548
Sum of electronic and thermal Enthalpies= -298.195604
Sum of electronic and thermal Free Energies= -298.239723

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	115.488	35.606	92.857

6d-9 Product
B3LYP/6-31+G**
E(RB3LYP) = -298.420047986

Zero-point correction= 0.174508 (Hartree/Particle)
Thermal correction to Energy= 0.184099
Thermal correction to Enthalpy= 0.185043
Thermal correction to Gibbs Free Energy= 0.140951
Sum of electronic and ZPE= -298.245540
Sum of electronic and thermal Energies= -298.235949
Sum of electronic and thermal Enthalpies= -298.235005
Sum of electronic and thermal Free Energies= -298.279097

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	115.524	34.611	92.799

C,0,0.1400279169,-1.4558740144,3.6390753011
C,0,1.587968283,-0.9975179825,3.8730640144
C,0,2.0744875719,-0.080425363,2.7126746991
O,0,1.1274821374,0.9611748761,2.400327757
C,0,1.0384182082,1.9938787285,3.3640734565
C,0,2.509707424,-2.21127958,4.0739352159
B,0,3.5684610805,0.3828401854,2.6550675471
H,0,2.0533152428,-0.7175130806,1.799676858
H,0,4.4484566959,-0.4041995604,2.8321970926
H,0,3.8532901333,1.4948638256,2.3260964895
H,0,1.6115515627,-0.4078915663,4.8007581325
H,0,-0.2262236543,-2.0290714904,4.4982007575
H,0,-0.5315007277,-0.6097726945,3.4742616716
H,0,0.0790929768,-2.1018051059,2.7536791577
H,0,0.416637734,2.7801065342,2.9286455717
H,0,0.5692857933,1.6537336595,4.2989735067
H,0,2.0272491432,2.4166611726,3.5991166564
H,0,2.1000720432,-2.8705319114,4.8468571137
H,0,2.5931710323,-2.7998418856,3.1513358359
H,0,3.5197644025,-1.9254797467,4.3790231651

B3LYP/6-31G*
E(RB3LYP) = -298.392684753

Zero-point correction= 0.175829 (Hartree/Particle)
Thermal correction to Energy= 0.185357
Thermal correction to Enthalpy= 0.186301
Thermal correction to Gibbs Free Energy= 0.142378
Sum of electronic and ZPE= -298.216855
Sum of electronic and thermal Energies= -298.207327
Sum of electronic and thermal Enthalpies= -298.206383
Sum of electronic and thermal Free Energies= -298.250306

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	116.313	34.349	92.444

C,0,0.1405153018,-1.4519444926,3.6366282677
C,0,1.5882543305,-0.9965665961,3.8729570777
C,0,2.0715904722,-0.0803989129,2.7106483577
O,0,1.1249517886,0.9574628848,2.3998766968
C,0,1.0406712559,1.9833196648,3.3664023149
C,0,2.5091587857,-2.2094393168,4.0744750963
B,0,3.565619586,0.3862591328,2.6535841424

H,0,2.0496505831,-0.7215853217,1.8005708951
H,0,4.4505433324,-0.3964479149,2.8332145945
H,0,3.8501060369,1.4986741818,2.3211315369
H,0,1.6109716446,-0.4053560214,4.8000119181
H,0,-0.2359471552,-2.0129210455,4.5000690685
H,0,-0.5235042025,-0.6028002533,3.4556700898
H,0,0.0820259911,-2.1093418709,2.7588294059
H,0,0.4187544238,2.7736366767,2.936289371
H,0,0.5736732985,1.6440810751,4.3036736611
H,0,2.030259543,2.405526145,3.6035473042
H,0,2.1012465445,-2.8685730347,4.8493599972
H,0,2.5921138624,-2.7996213391,3.1522907217
H,0,3.5200595767,-1.9219086411,4.3778094826

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.168794	E(Thermal)=	0.178606
E(QCISD(T))=	-297.424582	E(Empiric)=	-0.141960
DE(Plus)=	-0.018255	DE(2DF)=	-0.288112
E(Delta-G3)=	-0.403948	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.108064	G3 Energy=	-298.098252
G3 Enthalpy=	-298.097308	G3 Free Energy=	-298.141798

6d-10 Product
B3LYP/6-31G**
E(RB3LYP) = -298.423145214

Zero-point correction=	0.175003 (Hartree/Particle)
Thermal correction to Energy=	0.184362
Thermal correction to Enthalpy=	0.185306
Thermal correction to Gibbs Free Energy=	0.142168
Sum of electronic and zero-point Energies=	-298.248142
Sum of electronic and thermal Energies=	-298.238783
Sum of electronic and thermal Enthalpies=	-298.237839
Sum of electronic and thermal Free Energies=	-298.280977

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	115.689	34.359	90.793

O,0,1.5524659093,0.6682758616,1.4816644598
C,0,2.1455791165,-0.533538127,1.9492404086
C,0,2.0074443328,-0.7398380313,3.4812444352

C,0,0.5174147847,-0.7463330358,3.870629949
C,0,2.2363909911,1.8239186613,1.8883194026
B,0,2.8710831649,0.3089722929,4.2764061517
H,0,1.6174274975,-1.336953002,1.4208595284
H,0,3.2085222573,-0.5701902996,1.6571689353
H,0,2.434413164,0.9115635664,5.2161834212
H,0,4.0298193902,0.4485913896,4.0003577626
C,0,2.6444520299,-2.1223199771,3.8040901803
H,0,0.3917989039,-0.8941578979,4.949344577
H,0,0.0367597542,0.1995608586,3.6019990237
H,0,-0.0261383606,-1.5505156558,3.3551336506
H,0,1.6973096681,2.6856445303,1.4856138426
H,0,2.2559965702,1.9339630015,2.9956936856
H,0,3.2773355374,1.840654833,1.531096322
H,0,2.5906658437,-2.3532642097,4.8744684074
H,0,2.1017611077,-2.9177387108,3.2744830941
H,0,3.6970823374,-2.1731150483,3.5024587624

B3LYP/6-31G*
E(RB3LYP) = -298.396077006

Zero-point correction= 0.176317 (Hartree/Particle)
Thermal correction to Energy= 0.185597
Thermal correction to Enthalpy= 0.186541
Thermal correction to Gibbs Free Energy= 0.143595
Sum of electronic and zero-point Energies= -298.219760
Sum of electronic and thermal Energies= -298.210480
Sum of electronic and thermal Enthalpies= -298.209536
Sum of electronic and thermal Free Energies= -298.252482

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	116.464	34.074	90.388

O,0,1.5524659093,0.6682758616,1.4816644598
C,0,2.1455791165,-0.533538127,1.9492404086
C,0,2.0074443328,-0.739380313,3.4812444352
C,0,0.5174147847,-0.7463330358,3.870629949
C,0,2.2363909911,1.8239186613,1.8883194026
B,0,2.8710831649,0.3089722929,4.2764061517
H,0,1.6174274975,-1.336953002,1.4208595284
H,0,3.2085222573,-0.5701902996,1.6571689353
H,0,2.434413164,0.9115635664,5.2161834212
H,0,4.0298193902,0.4485913896,4.0003577626

C,0,2.6444520299,-2.1223199771,3.8040901803
H,0,0.3917989039,-0.8941578979,4.949344577
H,0,0.0367597542,0.1995608586,3.6019990237
H,0,-0.0261383606,-1.5505156558,3.3551336506
H,0,1.6973096681,2.6856445303,1.4856138426
H,0,2.2559965702,1.9339630015,2.9956936856
H,0,3.2773355374,1.840654833,1.531096322
H,0,2.5906658437,-2.3532642097,4.8744684074
H,0,2.1017611077,-2.9177387108,3.2744830941
H,0,3.6970823374,-2.1731150483,3.5024587624

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.169264	E(Thermal)=	0.178832
E(QCISD(T))=	-297.429582	E(Empiric)=	-0.141960
DE(Plus)=	-0.018898	DE(2DF)=	-0.289179
E(Delta-G3)=	-0.403209	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.113564	G3 Energy=	-298.103996
G3 Enthalpy=	-298.103052	G3 Free Energy=	-298.146555

6d-11 Product
B3LYP/6-31+G**
E(RB3LYP) = -298.421817199

Zero-point correction= 0.174353 (Hartree/Particle)
Thermal correction to Energy= 0.184130
Thermal correction to Enthalpy= 0.185074
Thermal correction to Gibbs Free Energy= 0.140081
Sum of electronic and ZPE= -298.247464
Sum of electronic and thermal Energies= -298.237687
Sum of electronic and thermal Enthalpies= -298.236743
Sum of electronic and thermal Free Energies= -298.281736

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	115.543	34.654	94.696

C,0,1.6227416426,-0.0158324932,1.0074608148
C,0,2.7923781086,-0.2365514752,1.9799416511
C,0,2.267948867,-0.7120415174,3.3707406928
O,0,1.317112905,0.2747446122,3.8142797392
H,0,0.8862829891,0.6742493158,1.4236438771
B,0,3.4144506621,-0.9956763883,4.4083731053

C,0,3.8174816579,-1.2103908302,1.3756358586
H,0,1.1181372013,-0.9664249502,0.7900035588
H,0,1.9880908156,0.3937182527,0.0587832483
H,0,3.2839578501,0.7335143033,2.1383488139
H,0,3.5211955249,-0.3421336006,5.4030121187
H,0,4.1979935969,-1.8760001722,4.2151083652
H,0,1.7248583223,-1.6639241286,3.183393708
C,0,0.4957766511,-0.1634667378,4.876365434
H,0,-0.1792675296,0.659564437,5.1236358576
H,0,-0.1025669784,-1.0424153221,4.5850820695
H,0,1.0802323838,-0.4204441157,5.7738025675
H,0,4.0873680723,-0.888076929,0.3643205706
H,0,4.7388289655,-1.2736120543,1.961351982
H,0,3.4025082917,-2.2231192061,1.2982639671

B3LYP/6-31G*
E(RB3LYP) = -298.394506350

Zero-point correction= 0.175684 (Hartree/Particle)
Thermal correction to Energy= 0.185417
Thermal correction to Enthalpy= 0.186361
Thermal correction to Gibbs Free Energy= 0.141511
Sum of electronic and ZPE= -298.218822
Sum of electronic and thermal Energies= -298.209090
Sum of electronic and thermal Enthalpies= -298.208146
Sum of electronic and thermal Free Energies= -298.252995

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	116.351	34.405	94.394

C,0,1.621333841,-0.0124081924,1.0140255024
C,0,2.7910704052,-0.2402551928,1.9833719946
C,0,2.2597891044,-0.7204594883,3.3709042295
O,0,1.31682282,0.2701674489,3.8120689537
H,0,0.8833155716,0.6684558917,1.4430219694
B,0,3.4190364141,-0.9833416089,4.4011943235
C,0,3.8143828599,-1.2133476299,1.3775649599
H,0,1.1196017268,-0.9622091643,0.7849803412
H,0,1.9828810104,0.411338915,0.0694706358
H,0,3.2840163263,0.7284173939,2.147577796
H,0,3.5706659054,-0.271744603,5.350654441
H,0,4.174958184,-1.8964732309,4.2453750952
H,0,1.7176658165,-1.6711371029,3.1814059785

C,0,0.4982455801,-0.1716237897,4.869106778
H,0,-0.1739330481,0.652201865,5.1254103528
H,0,-0.1064126805,-1.047965352,4.5791028292
H,0,1.0813759195,-0.4392428193,5.7662001028
H,0,4.0926907654,-0.8859203991,0.3694394093
H,0,4.7324928074,-1.2845986573,1.9692362732
H,0,3.3955106706,-2.2241732837,1.291436034

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.168657	E(Thermal)=	0.178665
E(QCISD(T))=	-297.426531	E(Empiric)=	-0.141960
DE(Plus)=	-0.018405	DE(2DF)=	-0.287478
E(Delta-G3)=	-0.403787	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.109504	G3 Energy=	-298.099496
G3 Enthalpy=	-298.098552	G3 Free Energy=	-298.143963

6d-12 Product
B3LYP/6-31+G**
E(RB3LYP) = -298.425575649

Zero-point correction= 0.174402 (Hartree/Particle)
Thermal correction to Energy= 0.184274
Thermal correction to Enthalpy= 0.185219
Thermal correction to Gibbs Free Energy= 0.140459
Sum of electronic and ZPE= -298.251174
Sum of electronic and thermal Energies= -298.241301
Sum of electronic and thermal Enthalpies= -298.240357
Sum of electronic and thermal Free Energies= -298.285116

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	115.634	34.873	94.204

C,0,0.6510184634,-0.5047173497,4.0387933893
C,0,2.045662036,-0.9461141999,3.5053073322
B,0,3.0372292279,0.1298968809,4.0887521081
C,0,2.3449741716,-2.3843232236,3.9733967037
C,0,2.0305654296,-0.8710848796,1.9745990701
O,0,3.3581385329,-1.0860886952,1.5040815192
C,0,3.4707554336,-1.027854432,0.0947135482
H,0,1.6757711394,0.1185242342,1.6417099102
H,0,1.3558100227,-1.6339956645,1.5451832963
H,0,3.6329341383,-0.0652702527,5.1088575355

H,0,3.1279252958,1.20326356,3.5671374998
H,0,0.610457419,-0.5457273074,5.1329308457
H,0,0.3854958994,0.5117380287,3.7262534339
H,0,-0.1252905408,-1.1838987906,3.661545641
H,0,4.5195934282,-1.2052041811,-0.1538857617
H,0,2.8515563021,-1.799163821,-0.3889913371
H,0,3.1708730976,-0.0418330445,-0.292689893
H,0,2.3640024358,-2.4440856892,5.0669443342
H,0,1.5807018718,-3.0853264896,3.6099991208
H,0,3.3148051956,-2.7252626832,3.5996377038

B3LYP/6-31G*
E(RB3LYP) = -298.403145769

Zero-point correction= 0.177542 (Hartree/Particle)
Thermal correction to Energy= 0.186424
Thermal correction to Enthalpy= 0.187368
Thermal correction to Gibbs Free Energy= 0.145117
Sum of electronic and ZPE= -298.225604
Sum of electronic and thermal Energies= -298.216722
Sum of electronic and thermal Enthalpies= -298.215778
Sum of electronic and thermal Free Energies= -298.258029

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	116.983	33.101	88.926

C,0,0.6707676324,-0.3683797872,4.0138777222
C,0,1.8796070239,-1.1315924353,3.4624392497
B,0,3.2572722921,-0.2792637776,3.2286298116
C,0,2.0833578399,-2.4530407835,4.2198837434
C,0,1.822029581,-1.357026434,1.9467782621
O,0,3.2516870633,-1.090307151,1.6924936269
C,0,3.6069320376,-0.4599786394,0.461472036
H,0,1.2290208936,-0.6007613646,1.4187562584
H,0,1.5774352167,-2.3575436545,1.568857257
H,0,4.2771219638,-0.5790948621,3.7907520072
H,0,3.1211096333,0.8885506934,2.9475928515
H,0,0.8297261687,-0.1123405035,5.0684755463
H,0,0.5043056608,0.5707693526,3.4732511211
H,0,-0.2554724709,-0.9601564197,3.9629154757
H,0,4.6828419113,-0.280621774,0.4993800017
H,0,3.369312813,-1.1302118369,-0.3710848515
H,0,3.0750176309,0.4921435325,0.3491871066

H,0,2.3102811501,-2.2590778119,5.2748886007
H,0,1.1876384046,-3.0917971451,4.1857718216
H,0,2.922986554,-3.0267971977,3.8099583519

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.170440	E(Thermal)=	0.179608
E(QCISD(T))=	-297.439226	E(Empiric)=	-0.141960
DE(Plus)=	-0.018106	DE(2DF)=	-0.288732
E(Delta-G3)=	-0.401568	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.119152	G3 Energy=	-298.109984
G3 Enthalpy=	-298.109040	G3 Free Energy=	-298.151830

6d-13 product
B3LYP/6-31+G**
E(RB3LYP) = -298.427884807

Zero-point correction= 0.176244 (Hartree/Particle)
Thermal correction to Energy= 0.185410
Thermal correction to Enthalpy= 0.186354
Thermal correction to Gibbs Free Energy= 0.143214
Sum of electronic and ZPE= -298.251640
Sum of electronic and thermal Energies= -298.242475
Sum of electronic and thermal Enthalpies= -298.241531
Sum of electronic and thermal Free Energies= -298.284671

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	116.346	33.653	90.795

C,0,1.4878448617,-0.2112297124,1.0897553071
C,0,2.7524499694,-0.1739430665,1.9568648665
C,0,2.5099225283,-0.8390490388,3.3248464852
C,0,3.2926148593,1.2251041435,2.2072409501
H,0,4.232879582,1.1984210502,2.7644875688
O,0,3.5336945399,1.9944139945,0.9191182843
C,0,4.8537881852,2.5194936025,0.7094384056
H,0,1.6446417783,0.2950648405,0.132795168
H,0,0.6487260025,0.2781566958,1.5945119933
H,0,1.2033483818,-1.2491661011,0.8835496284
H,0,3.5359468681,-0.7514040271,1.4401832071
B,0,2.5436092231,2.6022380792,2.127759602
H,0,4.780095556,3.2422069593,-0.1060545224

H,0,5.222268804,3.0176341825,1.6116375519
H,0,5.5202561976,1.698913905,0.426990618
H,0,2.1702575581,-1.8718657117,3.1938426937
H,0,3.4204345237,-0.8612879634,3.9349980274
H,0,1.7397260117,-0.3000393013,3.8884261964
H,0,3.0548622292,3.5553715074,2.6437396281
H,0,1.4199293401,2.6749439621,1.7319063405

E(RB3LYP) = -298.402106260

Zero-point correction= 0.177652 (Hartree/Particle)
Thermal correction to Energy= 0.186734
Thermal correction to Enthalpy= 0.187678
Thermal correction to Gibbs Free Energy= 0.144727
Sum of electronic and ZPE= -298.224455
Sum of electronic and thermal Energies= -298.215372
Sum of electronic and thermal Enthalpies= -298.214428
Sum of electronic and thermal Free Energies= -298.257380

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	117.177	33.352	90.399

C,0,1.496013198,-0.2066360004,1.0863719812
C,0,2.7570790872,-0.1764092256,1.9578241737
C,0,2.5065225131,-0.8380547492,3.3250111332
C,0,3.3008904407,1.2210394086,2.2076281144
H,0,4.24906053,1.1909885062,2.751792372
O,0,3.5239605457,1.9900305084,0.9176359557
C,0,4.8381018512,2.5204504294,0.705034234
H,0,1.6645927889,0.2918531637,0.1267369831
H,0,0.6602719699,0.2967347725,1.5836033767
H,0,1.2001222436,-1.2430088312,0.8855561685
H,0,3.5388740178,-0.7590416387,1.4436858997
B,0,2.5497486771,2.5964422825,2.1410060942
H,0,4.7604335934,3.2414857052,-0.1122237351
H,0,5.2085152702,3.0226873608,1.6044620391
H,0,5.5101963687,1.7037796024,0.4220074533
H,0,2.1592611094,-1.8690264011,3.1946703278
H,0,3.416183696,-0.8662402241,3.9373363789
H,0,1.7395799581,-0.2919663682,3.8868966024
H,0,3.0677034563,3.549650364,2.6524772636
H,0,1.4201856847,2.6692193349,1.7585251838

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.170546	E(Thermal)=	0.179910
E(QCISD(T))=	-297.436923	E(Empiric)=	-0.141960
DE(Plus)=	-0.017277	DE(2DF)=	-0.288038
E(Delta-G3)=	-0.403088	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.116740	G3 Energy=	-298.107376
G3 Enthalpy=	-298.106432	G3 Free Energy=	-298.149926

6d-14 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -298.384129826

Zero-point correction= 0.169252 (Hartree/Particle)
Thermal correction to Energy= 0.180454
Thermal correction to Enthalpy= 0.181398
Thermal correction to Gibbs Free Energy= 0.131405
Sum of electronic and zero-point Energies= -298.214877
Sum of electronic and thermal Energies= -298.203676
Sum of electronic and thermal Enthalpies= -298.202732
Sum of electronic and thermal Free Energies= -298.252725

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	113.236	36.757	105.218

B3LYP/6-31+G*
E(RB3LYP) = -298.357018345

Zero-point correction= 0.170304 (Hartree/Particle)
Thermal correction to Energy= 0.181680
Thermal correction to Enthalpy= 0.182624
Thermal correction to Gibbs Free Energy= 0.130620
Sum of electronic and ZPE= -298.186715
Sum of electronic and thermal Energies= -298.175338
Sum of electronic and thermal Enthalpies= -298.174394
Sum of electronic and thermal Free Energies= -298.226399

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	114.006	36.665	109.453

C,0,-0.21902,0.20614,-0.88305
C,0,-0.45139,-0.81,-0.02455
C,0,-0.93998,-0.78189,1.40588
C,0,-0.68487,2.21576,0.39917
B,0,2.98507,-0.15226,0.10753
H,0,0.0974,-0.03553,-1.89465
H,0,3.21157,-0.94631,-0.75533
H,0,2.96274,1.01426,-0.14511
H,0,2.84368,-0.5233,1.23443
C,0,-0.2866,-2.21635,-0.56521
H,0,-0.66083,3.28431,0.1724
H,0,-1.69603,1.94265,0.72458
H,0,0.03157,2.00438,1.20235
H,0,-0.26385,-1.36657,2.0443
H,0,-1.02835,0.20974,1.84524
H,0,-1.92445,-1.26677,1.47696
H,0,0.42614,-2.79598,0.03717
H,0,-1.24224,-2.75972,-0.52958
H,0,0.06458,-2.22628,-1.60143
O,0,-0.3218,1.56147,-0.80501

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.163491	E(Thermal)=	0.175119
E(QCISD(T))=	-297.383870	E(Empiric)=	-0.141960
DE(Plus)=	-0.018765	DE(2DF)=	-0.286184
E(Delta-G3)=	-0.405096	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.072383	G3 Energy=	-298.060755
G3 Enthalpy=	-298.059811	G3 Free Energy=	-298.112421

6d-15 Variational Transtion State
B3LYP/6-31+G**
E(RB3LYP) = -298.395666120

Zero-point correction=	0.169641 (Hartree/Particle)
Thermal correction to Energy=	0.180311
Thermal correction to Enthalpy=	0.181255
Thermal correction to Gibbs Free Energy=	0.134164
Sum of electronic and zero-point Energies=	-298.226025
Sum of electronic and thermal Energies=	-298.215355
Sum of electronic and thermal Enthalpies=	-298.214411
Sum of electronic and thermal Free Energies=	-298.261502

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	113.147	36.316	99.111

B3LYP/6-31+G*
E(RB3LYP) = -298.368735277

Zero-point correction= 0.170672 (Hartree/Particle)
Thermal correction to Energy= 0.180582
Thermal correction to Enthalpy= 0.181527
Thermal correction to Gibbs Free Energy= 0.136289
Sum of electronic and ZPE= -298.198063
Sum of electronic and thermal Energies= -298.188153
Sum of electronic and thermal Enthalpies= -298.187209
Sum of electronic and thermal Free Energies= -298.232447

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	113.317	34.242	95.211

C,0,-1.67573,0.04182,1.25756
C,0,-0.95877,0.43418,-0.00761
C,0,0.03747,-0.31666,-0.52242
O,0,0.41705,-1.49947,0.04149
H,0,-1.18102,-0.79026,1.7605
B,0,1.8181,1.68546,0.3189
C,0,-1.49498,1.62314,-0.76036
H,0,-2.70908,-0.25903,1.03199
H,0,-1.73871,0.88917,1.95284
H,0,2.28887,0.91452,1.10108
H,0,2.19541,1.68641,-0.81599
H,0,1.10922,2.56414,0.70655
H,0,0.50262,-0.07887,-1.47953
C,0,1.71139,-1.959,-0.32651
H,0,1.81538,-2.96223,0.09238
H,0,1.81834,-2.01192,-1.41929
H,0,2.49359,-1.30741,0.08019
H,0,-1.49977,2.5223,-0.13153
H,0,-0.90952,1.84319,-1.65898
H,0,-2.53519,1.44626,-1.06981

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.163845	E(Thermal)=	0.174020
E(QCISD(T))=	-297.395909	E(Empiric)=	-0.141960

DE(Plus)=	-0.018716	DE(2DF)=	-0.286378
E(Delta-G3)=	-0.404830	E(G3-Empiric)=	-0.141960
G3(0 K)=	-298.083948	G3 Energy=	-298.073773
G3 Enthalpy=	-298.072829	G3 Free Energy=	-298.118626

6e-1 Starting Material
B3LYP/6-31+G**
E(RB3LYP) = -311.086915774

Zero-point correction= 0.169461 (Hartree/Particle)
Thermal correction to Energy= 0.177706
Thermal correction to Enthalpy= 0.178651
Thermal correction to Gibbs Free Energy= 0.137239
Sum of electronic and ZPE= -310.917455
Sum of electronic and thermal Energies= -310.909209
Sum of electronic and thermal Enthalpies= -310.908265
Sum of electronic and thermal Free Energies= -310.949676

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.512	29.851	87.157

O,0,2.2120666317,0.7234136784,1.2900298086
C,0,2.4510970814,-0.4160962176,2.0079401533
C,0,1.987978233,-0.9067688802,3.1743121194
C,0,0.985870371,-0.3269249777,4.1468069692
C,0,1.2864467395,1.722665079,1.717226528
H,0,3.1820433329,-0.998844216,1.4543708034
C,0,2.5328694216,-2.2498292145,3.6194640422
C,0,1.2810430316,2.8185122721,0.6644294193
H,0,0.2862938528,1.2820507547,1.8220088409
H,0,1.5959364781,2.1242295594,2.691071738
H,0,0.5816342597,3.6104847138,0.9527290851
H,0,2.2777023645,3.2572048626,0.5576934995
H,0,0.9735198454,2.4201017331,-0.3070956709
H,0,3.0279813247,-2.1696358439,4.5971127783
H,0,1.7238118501,-2.9841487769,3.735951064
H,0,3.257615489,-2.6609289122,2.910540951
H,0,1.4478948138,-0.2112765019,5.1369576508
H,0,0.5728435991,0.637740897,3.8620915931
H,0,0.1456502796,-1.0223240089,4.2797866269

B3LYP/6-31G*
E(RB3LYP) = -311.059275090

Zero-point correction= 0.170891 (Hartree/Particle)
Thermal correction to Energy= 0.179969
Thermal correction to Enthalpy= 0.180913
Thermal correction to Gibbs Free Energy= 0.135799
Sum of electronic and ZPE= -310.888384
Sum of electronic and thermal Energies= -310.879306
Sum of electronic and thermal Enthalpies= -310.878362
Sum of electronic and thermal Free Energies= -310.923476

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.932	31.516	94.951

O,0,2.2108313704,0.7243862504,1.291383508
C,0,2.4470673304,-0.4113715776,2.0097897396
C,0,1.9864573864,-0.9037335786,3.1737363476
C,0,0.9851771001,-0.3268108919,4.1474018098
C,0,1.2871491028,1.7196879286,1.7196791995
H,0,3.1786919952,-0.9943492332,1.4555027207
C,0,2.5334417931,-2.2458302714,3.6147989799
C,0,1.2831176143,2.8144239855,0.6648031481
H,0,0.2851352478,1.2825792197,1.8276040406
H,0,1.5926559986,2.1235111024,2.6945573908
H,0,0.5853898371,3.6102871458,0.9478150559
H,0,2.282082122,3.2489243648,0.5576992944
H,0,0.9772341556,2.4119780562,-0.3060956468
H,0,3.0300488456,-2.1699792334,4.5932381497
H,0,1.7267331936,-2.9841700114,3.732239105
H,0,3.258600881,-2.6552066363,2.9040621154
H,0,1.4457996276,-0.2115757199,5.1393184545
H,0,0.5709128487,0.6389292871,3.8641571414
H,0,0.1437725495,-1.0220541866,4.281737446

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.164055	E(Thermal)=	0.173379
E(QCISD(T))=	-310.081410	E(Empiric)=	-0.141960
DE(Plus)=	-0.018227	DE(2DF)=	-0.286352
E(Delta-G3)=	-0.413051	E(G3-Empiric)=	-0.141960
G3(0 K)=	-310.776945	G3 Energy=	-310.767621
G3 Enthalpy=	-310.766677	G3 Free Energy=	-310.812297

For Anharmonic Corrections of 6e-1

Zero-point vibrational energy 448674.4 (Joules/Mol)
107.23575 (Kcal/Mol)
Warning -- explicit consideration of 11 degrees of freedom as vibrations may cause significant error
Vibrational temperatures: 12.44 159.44 247.98 265.61 303.40
(Kelvin) 365.73 440.98 464.15 502.44 585.39
657.48 980.54 1174.00 1230.62 1282.78
1285.50 1415.79 1474.35 1490.67 1559.28
1602.19 1652.92 1719.40 1753.61 1825.60
1885.48 2036.95 2070.85 2078.75 2081.42
2108.15 2162.19 2177.64 2188.73 2191.16
2202.46 2207.46 2242.27 2513.20 4338.40
4346.29 4352.39 4395.68 4398.08 4403.81
4407.50 4483.98 4505.86 4516.87 4585.57
4592.70

Zero-point correction= 0.170891 (Hartree/Particle)
Thermal correction to Energy= 0.179970
Thermal correction to Enthalpy= 0.180914
Thermal correction to Gibbs Free Energy= 0.135786
Sum of electronic and zero-point Energies= -310.888384
Sum of electronic and thermal Energies= -310.879305
Sum of electronic and thermal Enthalpies= -310.878361
Sum of electronic and thermal Free Energies= -310.923490

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	112.933	31.516	94.981

ZPE(harm) = 0.44867D+03 kJ/mol ZPE(anh)= 0.44201D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.30143D-75	0.18747D-74	
QZvib	0.12118D+04	0.51247D+03	
Energy	0.47251D+03	0.46589D+03	kJ/mol
Enthalpy	0.47499D+03	0.46837D+03	kJ/mol
Entropy	0.39740D+03	0.39038D+03	J/(mol K)
Sp.Heat(V)	0.13187D+03	0.13366D+03	J/(mol K)
Sp.Heat(P)	0.14018D+03	0.14197D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.30143D-75	0.18747D-74	
QZvib	0.12118D+04	0.51247D+03	
Energy	0.47251D+03	0.46589D+03	kJ/mol
Enthalpy	0.47499D+03	0.46837D+03	kJ/mol
Entropy	0.39740D+03	0.39038D+03	J/(mol K)
Sp.Heat(V)	0.13187D+03	0.13366D+03	J/(mol K)
Sp.Heat(P)	0.14018D+03	0.14197D+03	J/(mol K)

6e-2 Starting Material

B3LYP/6-31G**

E(RB3LYP) = -311.095236281

Zero-point correction= 0.168856 (Hartree/Particle)
Thermal correction to Energy= 0.178160
Thermal correction to Enthalpy= 0.179104
Thermal correction to Gibbs Free Energy= 0.134515
Sum of electronic and zero-point Energies= -310.926381
Sum of electronic and thermal Energies= -310.917076
Sum of electronic and thermal Enthalpies= -310.916132
Sum of electronic and thermal Free Energies= -310.960721

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.797	32.067	93.846

O,0,0.894276106,0.4919897641,2.678687081
C,0,1.8833740966,-0.4569696025,2.7503584792
C,0,1.8443762659,-1.4895370502,3.6049080414
C,0,0.735882703,-1.6722479277,4.6079334543
C,0,1.2979576969,1.7495933264,2.1299200774
H,0,2.6921236244,-0.338188537,2.02821191
C,0,2.921883092,-2.5434731503,3.5718716727
H,0,1.7835301066,1.5837734475,1.1560540772
C,0,0.0664205538,2.6237487791,1.9748388971
H,0,2.0336087994,2.221895927,2.7974731929
H,0,3.415402555,-2.6338316978,4.5490397773
H,0,2.5034312093,-3.5322355836,3.3383192306
H,0,3.69096061,-2.3214831341,2.8248923511
H,0,1.1428724867,-1.7711459249,5.6233712002
H,0,0.0368092636,-0.8337745353,4.5934544633
H,0,0.1711672921,-2.5927076958,4.4048030406

H,0,0.346453145,3.5962138398,1.5561968937
H,0,-0.6598847585,2.1528893659,1.3054003641
H,0,-0.4148538478,2.7900193894,2.9433617958

B3LYP/6-31G*
E(RB3LYP) = -311.067043584

Zero-point correction= 0.170229 (Hartree/Particle)
Thermal correction to Energy= 0.179460
Thermal correction to Enthalpy= 0.180405
Thermal correction to Gibbs Free Energy= 0.136034
Sum of electronic and zero-point Energies= -310.896814
Sum of electronic and thermal Energies= -310.887583
Sum of electronic and thermal Enthalpies= -310.886639
Sum of electronic and thermal Free Energies= -310.931009

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	112.613	31.777	93.385

O,0,0.8874690107,0.4768794541,2.6547065233
C,0,1.8775966894,-0.4668307921,2.737036802
C,0,1.844690846,-1.4857354598,3.6047009185
C,0,0.7425124886,-1.6488863924,4.617606593
C,0,1.2979444825,1.7402639331,2.1352075357
H,0,2.6843403106,-0.3551255533,2.0100228335
C,0,2.9225564304,-2.5378796818,3.578972163
H,0,1.8125014469,1.5951647898,1.1720262826
C,0,0.0619594856,2.6048368283,1.9591194206
H,0,2.0131330647,2.2139897644,2.824444657
H,0,3.4241267468,-2.6169946385,4.5541137271
H,0,2.5068914115,-3.5323722689,3.3610465978
H,0,3.687402487,-2.3246976516,2.8239810638
H,0,1.1536257066,-1.7382051387,5.6331516698
H,0,0.0513571391,-0.803252528,4.5960827569
H,0,0.1660222087,-2.5666162617,4.4322842131
H,0,0.339012914,3.5865913153,1.5597386732
H,0,-0.6420350514,2.1322815905,1.266743017
H,0,-0.445316818,2.7511176914,2.9181105519

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.163420 E(Thermal)= 0.172896

E(QCISD(T))=	-310.089553	E(Empiric)=	-0.141960
DE(Plus)=	-0.018991	DE(2DF)=	-0.285488
E(Delta-G3)=	-0.412260	E(G3-Empiric)=	-0.141960
G3(0 K)=	-310.784832	G3 Energy=	-310.775356
G3 Enthalpy=	-310.774412	G3 Free Energy=	-310.819293

6e-3 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -311.083971025

Zero-point correction= 0.169712 (Hartree/Particle)
Thermal correction to Energy= 0.178748
Thermal correction to Enthalpy= 0.179692
Thermal correction to Gibbs Free Energy= 0.135753
Sum of electronic and ZPE= -310.914259
Sum of electronic and thermal Energies= -310.905224
Sum of electronic and thermal Enthalpies= -310.904279
Sum of electronic and thermal Free Energies= -310.948218

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.166	31.775	92.476

O,0,2.0160718013,0.6298582312,1.5143335231
C,0,2.208257269,-0.553795791,2.1739506061
C,0,1.7847455066,-1.0704828981,3.3443065192
C,0,0.8761273695,-0.4834387621,4.400151181
C,0,1.142631494,1.6635207477,1.9772444802
H,0,2.8756437491,-1.1534584029,1.5608798456
C,0,2.2928152529,-2.4525249355,3.7068032093
H,0,1.4411629243,-0.2768037535,5.3198919345
H,0,0.3683426351,0.4353910637,4.1146342069
H,0,0.1029540668,-1.2146237166,4.6726279425
H,0,1.4830973227,2.5558434587,1.4433321315
C,0,-0.319999212,1.3876378385,1.6429124262
H,0,1.2980266115,1.8430913901,3.046413701
H,0,2.8367232453,-2.4345474127,4.661599541
H,0,1.4606548979,-3.1592130033,3.8319477822
H,0,2.9670269617,-2.8602951701,2.9478502682
H,0,-0.9436228464,2.2267766305,1.9725679331
H,0,-0.4441014782,1.2715788704,0.5619272674
H,0,-0.686040571,0.4779776152,2.127025501

B3LYP/6-31G*
E(RB3LYP) = -311.056405607

Zero-point correction= 0.171098 (Hartree/Particle)
Thermal correction to Energy= 0.180054
Thermal correction to Enthalpy= 0.180998
Thermal correction to Gibbs Free Energy= 0.137274
Sum of electronic and ZPE= -310.885308
Sum of electronic and thermal Energies= -310.876352
Sum of electronic and thermal Enthalpies= -310.875408
Sum of electronic and thermal Free Energies= -310.919131

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.985	31.462	92.024

O,0,2.0065359548,0.6207752137,1.5060510873
C,0,2.199831299,-0.5551078743,2.1729017726
C,0,1.7813609383,-1.0701444354,3.3434953825
C,0,0.8701811391,-0.4881153426,4.3991875379
C,0,1.1472687031,1.6579335461,1.9759120829
H,0,2.8689913935,-1.1559241543,1.561422585
C,0,2.2985398695,-2.447190501,3.7071085493
H,0,1.4329278085,-0.2724479378,5.3192834048
H,0,0.3521816593,0.4256036077,4.1116674654
H,0,0.1030090418,-1.2248674911,4.6770306722
H,0,1.4912938774,2.552390512,1.4462691467
C,0,-0.318466016,1.3953273507,1.643959804
H,0,1.30465577,1.8335156327,3.0458459467
H,0,2.8456929964,-2.4267745306,4.6611429665
H,0,1.4719470655,-3.1609212042,3.8378955729
H,0,2.9734876351,-2.8536673242,2.9470101662
H,0,-0.9380605126,2.2388976273,1.9710002568
H,0,-0.4422339591,1.2753082396,0.5628618141
H,0,-0.6886276636,0.4879010658,2.130353786

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.164254	E(Thermal)=	0.173460
E(QCISD(T))=	-310.079030	E(Empiric)=	-0.141960
DE(Plus)=	-0.018519	DE(2DF)=	-0.286713
E(Delta-G3)=	-0.412572	E(G3-Empiric)=	-0.141960
G3(0 K)=	-310.774539	G3 Energy=	-310.765334
G3 Enthalpy=	-310.764390	G3 Free Energy=	-310.808618

For Anharmonic Corrections of 6e-3

Zero-point vibrational energy 449221.1 (Joules/Mol)
107.36641 (Kcal/Mol)
Warning -- explicit consideration of 11 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 50.80 131.54 219.58 291.30 327.96
(Kelvin) 415.11 436.99 460.99 560.61 617.66
675.64 920.71 1178.31 1188.24 1256.62
1287.13 1418.77 1448.76 1492.32 1555.62
1599.60 1617.68 1707.74 1768.99 1819.21
1921.34 2042.76 2071.33 2076.92 2085.37
2108.33 2161.51 2180.52 2184.62 2188.51
2204.80 2213.37 2234.23 2510.02 4338.10
4352.19 4395.34 4399.32 4400.55 4410.91
4463.63 4484.81 4498.43 4520.71 4577.45
4584.65

Zero-point correction= 0.171099 (Hartree/Particle)
Thermal correction to Energy= 0.180055
Thermal correction to Enthalpy= 0.180999
Thermal correction to Gibbs Free Energy= 0.137276
Sum of electronic and zero-point Energies= -310.885306
Sum of electronic and thermal Energies= -310.876351
Sum of electronic and thermal Enthalpies= -310.875407
Sum of electronic and thermal Free Energies= -310.919130

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	112.986	31.462	92.024

ZPE(harm) = 0.44922D+03 kJ/mol ZPE(anh)= 0.44099D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.64637D-76	0.46560D-75	
QZvib	0.32397D+03	0.84402D+02	
Energy	0.47273D+03	0.46312D+03	kJ/mol
Enthalpy	0.47521D+03	0.46559D+03	kJ/mol
Entropy	0.38503D+03	0.37750D+03	J/(mol K)
Sp.Heat(V)	0.13164D+03	0.12660D+03	J/(mol K)
Sp.Heat(P)	0.13995D+03	0.13491D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.64637D-76	0.46560D-75	
QZvib	0.32397D+03	0.84402D+02	
Energy	0.47273D+03	0.46312D+03	kJ/mol
Enthalpy	0.47521D+03	0.46559D+03	kJ/mol
Entropy	0.38503D+03	0.37750D+03	J/(mol K)
Sp.Heat(V)	0.13164D+03	0.12660D+03	J/(mol K)
Sp.Heat(P)	0.13995D+03	0.13491D+03	J/(mol K)

6e-4 Transition State

B3LYP/6-31+G**

E(RB3LYP) = -311.094358316

Zero-point correction= 0.168952 (Hartree/Particle)
Thermal correction to Energy= 0.178149
Thermal correction to Enthalpy= 0.179094
Thermal correction to Gibbs Free Energy= 0.134838
Sum of electronic and ZPE= -310.925407
Sum of electronic and thermal Energies= -310.916209
Sum of electronic and thermal Enthalpies= -310.915265
Sum of electronic and thermal Free Energies= -310.959521

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	111.790	32.033	93.145

C,0,1.7706130197,0.2143313133,1.1307780068
C,0,2.5997471289,-0.6905406498,2.0037714905
C,0,2.3589192896,-0.8526895179,3.3125925524
O,0,1.37910009,-0.1661221186,3.986075847
H,0,0.9259108826,0.6389403234,1.6768819435
C,0,3.7555917964,-1.405417404,1.3507948379
H,0,1.3850913945,-0.3322241936,0.2594105084
H,0,2.3757509813,1.0435791733,0.7387838196
H,0,2.969829644,-1.510388204,3.933015225
C,0,0.9108313878,-0.779979407,5.1912640301
H,0,0.4200132956,0.0233307356,5.7478575258
C,0,-0.057946598,-1.9275032474,4.9269115777
H,0,1.7721575174,-1.1236226668,5.7838544913
H,0,-0.4166526318,-2.3444649895,5.8750024235
H,0,-0.9220483757,-1.577051004,4.3539702448

H,0,0.4250612363,-2.7310447083,4.3614965521
H,0,4.480078645,-0.6925745831,0.9331307669
H,0,4.291037045,-2.0500055114,2.0555911508
H,0,3.4121232515,-2.0301583402,0.5150470062

B3LYP/6-31G*
E(RB3LYP) = -311.066603870

Zero-point correction= 0.170328 (Hartree/Particle)
Thermal correction to Energy= 0.179451
Thermal correction to Enthalpy= 0.180395
Thermal correction to Gibbs Free Energy= 0.136313
Sum of electronic and ZPE= -310.896276
Sum of electronic and thermal Energies= -310.887153
Sum of electronic and thermal Enthalpies= -310.886209
Sum of electronic and thermal Free Energies= -310.930291

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	112.607	31.729	92.779

C,0,1.753721624,0.1998139425,1.1455059592
C,0,2.6005957457,-0.6920048213,2.0144355063
C,0,2.3748701687,-0.8417494338,3.3254150082
O,0,1.4046456295,-0.150073325,4.0032713418
H,0,0.9076581704,0.6120613923,1.700055311
C,0,3.7512009836,-1.4089329948,1.3573949978
H,0,1.3668109477,-0.3520103138,0.277128637
H,0,2.3413211003,1.0388617838,0.7458533308
H,0,2.9930145413,-1.4944438773,3.9456861055
C,0,0.9211164682,-0.7779651955,5.1903857135
H,0,0.4294549534,0.0187575117,5.756881604
C,0,-0.0526183541,-1.9140681439,4.8970650365
H,0,1.7715473066,-1.1394124016,5.7894305753
H,0,-0.4296687808,-2.3459185278,5.8316456621
H,0,-0.9047669686,-1.5473172795,4.3154529053
H,0,0.4346482801,-2.7098669056,4.3232790514
H,0,4.4724474423,-0.6997912649,0.9256889816
H,0,4.2952268143,-2.0468644827,2.0628704914
H,0,3.4039829275,-2.0426806627,0.5287837814

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.163515	E(Thermal)=	0.172886
E(QCISD(T))=	-310.089436	E(Empiric)=	-0.141960

DE(Plus)=	-0.018801	DE(2DF)=	-0.285688
E(Delta-G3)=	-0.411960	E(G3-Empiric)=	-0.141960
G3(0 K)=	-310.784330	G3 Energy=	-310.774959
G3 Enthalpy=	-310.774015	G3 Free Energy=	-310.818608

For Anharmonic Corrections of 6e-4

Zero-point vibrational energy 447196.6 (Joules/Mol)
106.88255 (Kcal/Mol)
Warning -- explicit consideration of 12 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 65.22 116.03 221.09 253.10 291.97
(Kelvin) 356.14 418.77 467.83 570.14 614.65
709.02 790.84 1169.10 1216.94 1245.03
1301.18 1416.47 1478.67 1491.38 1563.95
1606.90 1620.27 1699.50 1772.89 1814.24
1934.48 2011.23 2042.04 2067.80 2079.34
2090.23 2162.77 2180.00 2181.25 2189.52
2192.20 2200.23 2217.94 2543.27 4332.07
4341.88 4352.90 4394.23 4402.10 4408.02
4464.73 4472.17 4495.02 4502.26 4511.21
4530.45

Zero-point correction= 0.170328 (Hartree/Particle)
Thermal correction to Energy= 0.179451
Thermal correction to Enthalpy= 0.180395
Thermal correction to Gibbs Free Energy= 0.136312
Sum of electronic and zero-point Energies= -310.896276
Sum of electronic and thermal Energies= -310.887153
Sum of electronic and thermal Enthalpies= -310.886209
Sum of electronic and thermal Free Energies= -310.930291

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	112.607	31.729	92.779

ZPE(harm) = 0.44720D+03 kJ/mol ZPE(anh)= 0.44012D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.16473D-75	0.38473D-74	
QZvib	0.36486D+03	0.48972D+03	
Energy	0.47115D+03	0.46440D+03	kJ/mol
Enthalpy	0.47363D+03	0.46688D+03	kJ/mol
Entropy	0.38819D+03	0.39176D+03	J/(mol K)

Sp.Heat(V)	0.13275D+03	0.13466D+03	J/(mol K)
Sp.Heat(P)	0.14107D+03	0.14298D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.16473D-75	0.38473D-74	
QZvib	0.36486D+03	0.48972D+03	
Energy	0.47115D+03	0.46440D+03	kJ/mol
Enthalpy	0.47363D+03	0.46688D+03	kJ/mol
Entropy	0.38819D+03	0.39176D+03	J/(mol K)
Sp.Heat(V)	0.13275D+03	0.13466D+03	J/(mol K)
Sp.Heat(P)	0.14107D+03	0.14298D+03	J/(mol K)

6e-5 Complex

B3LYP/6-31+G**

E(RB3LYP) = -337.720249958

Zero-point correction= 0.201669 (Hartree/Particle)
Thermal correction to Energy= 0.212835
Thermal correction to Enthalpy= 0.213779
Thermal correction to Gibbs Free Energy= 0.166276
Sum of electronic and zero-point Energies= -337.518581
Sum of electronic and thermal Energies= -337.507415
Sum of electronic and thermal Enthalpies= -337.506471
Sum of electronic and thermal Free Energies= -337.553974

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	133.556	40.709	99.978

O,0,2.2409188463,0.7243652317,1.3346568024
C,0,2.5776476007,-0.3322457907,2.0826421145
C,0,2.1779174892,-0.8066279381,3.3149519317
C,0,1.046326161,-0.2686168766,4.1730996133
C,0,1.31880909,1.7416338273,1.7680577295
B,0,3.8338726341,0.1896933683,3.7619542696
H,0,3.2739964243,-0.9395887505,1.5122998227
H,0,4.7952520656,-0.3359055812,3.2674343035
H,0,3.6705097959,1.3606358062,3.5351756911
H,0,3.6474885428,-0.1181399028,4.9126885583
C,0,2.5148035967,-2.2639439932,3.5990556895
C,0,1.1714620159,2.7207087453,0.6173415089
H,0,0.3580507264,1.2815368871,2.0230529313

H,0,1.7292609768,2.2321772333,2.655974297
H,0,0.4789608271,3.5216154909,0.8978336436
H,0,2.13789927,3.1686770767,0.3674661577
H,0,0.7801360958,2.219315638,-0.2734826944
H,0,2.7804892844,-2.3972539725,4.6521185981
H,0,1.6444194703,-2.8996449502,3.3856174242
H,0,3.352978225,-2.620405753,2.993302618
H,0,1.1933405323,-0.6015019536,5.204958662
H,0,0.9893729625,0.818916052,4.1912486729
H,0,0.080353367,-0.6655918945,3.8323786546

B3LYP/6-31+G*
E(RB3LYP) = -337.690601105

Zero-point correction= 0.203222 (Hartree/Particle)
Thermal correction to Energy= 0.214323
Thermal correction to Enthalpy= 0.215267
Thermal correction to Gibbs Free Energy= 0.167869
Sum of electronic and zero-point Energies= -337.487379
Sum of electronic and thermal Energies= -337.476278
Sum of electronic and thermal Enthalpies= -337.475334
Sum of electronic and thermal Free Energies= -337.522732

E (Thermal)	CV	S	
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin	Total
134.490	40.381	99.758	

O,0,2.2409188463,0.7243652317,1.3346568024
C,0,2.5776476007,-0.3322457907,2.0826421145
C,0,2.1779174892,-0.8066279381,3.3149519317
C,0,1.046326161,-0.2686168766,4.1730996133
C,0,1.31880909,1.7416338273,1.7680577295
B,0,3.8338726341,0.1896933683,3.7619542696
H,0,3.2739964243,-0.9395887505,1.5122998227
H,0,4.7952520656,-0.3359055812,3.2674343035
H,0,3.6705097959,1.3606358062,3.5351756911
H,0,3.6474885428,-0.1181399028,4.9126885583
C,0,2.5148035967,-2.2639439932,3.5990556895
C,0,1.1714620159,2.7207087453,0.6173415089
H,0,0.3580507264,1.2815368871,2.0230529313
H,0,1.7292609768,2.2321772333,2.655974297
H,0,0.4789608271,3.5216154909,0.8978336436
H,0,2.13789927,3.1686770767,0.3674661577
H,0,0.7801360958,2.219315638,-0.2734826944
H,0,2.7804892844,-2.3972539725,4.6521185981

H,0,1.6444194703,-2.8996449502,3.3856174242
H,0,3.352978225,-2.620405753,2.993302618
H,0,1.1933405323,-0.6015019536,5.204958662
H,0,0.9893729625,0.818916052,4.1912486729
H,0,0.080353367,-0.6655918945,3.8323786546

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.195093	E(Thermal)=	0.206530
E(QCISD(T))=	-336.588704	E(Empiric)=	-0.162240
DE(Plus)=	-0.019799	DE(2DF)=	-0.329248
E(Delta-G3)=	-0.460885	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.365784	G3 Energy=	-337.354346
G3 Enthalpy=	-337.353402	G3 Free Energy=	-337.401481

6e-6 Complex
B3LYP/6-31G**
E(RB3LYP) = -337.729993712

Zero-point correction= 0.201027 (Hartree/Particle)
Thermal correction to Energy= 0.212312
Thermal correction to Enthalpy= 0.213257
Thermal correction to Gibbs Free Energy= 0.165282
Sum of electronic and zero-point Energies= -337.528967
Sum of electronic and thermal Energies= -337.517681
Sum of electronic and thermal Enthalpies= -337.516737
Sum of electronic and thermal Free Energies= -337.564712

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	133.228	40.884	100.972

C,0,2.2293117125,0.5146801771,1.1920507172
C,0,2.674563842,-0.6409177157,2.0593772535
C,0,1.9331294062,-1.007691301,3.1553451524
O,0,0.7825523589,-0.3784124809,3.4797165696
H,0,1.72752145,1.2877171292,1.7761285897
B,0,3.655816062,0.0055991287,3.6826344796
C,0,3.6284524431,-1.6333761688,1.430668994
H,0,1.5246933992,0.1540328101,0.4310316069
H,0,3.0857509219,0.9599583555,0.6783023113
H,0,2.9966632263,0.6196141266,4.4799044592
H,0,4.3055424399,-0.9133691838,4.1016447555
H,0,4.2350957849,0.7351464657,2.9209885666

H,0,2.1417575775,-1.9302837332,3.6953691806
C,0,0.3310021681,-0.5431371422,4.8387366405
C,0,-1.0700878717,0.0280344065,4.9439988182
H,0,0.3450265575,-1.6129492387,5.0903499628
H,0,1.030538057,-0.0217017331,5.5020056015
H,0,4.5591604419,-1.1416473309,1.1324195718
H,0,3.8782377617,-2.4525553307,2.1094987142
H,0,3.1678406603,-2.0608057593,0.5304546368
H,0,-1.4365360311,-0.0781574008,5.9702358299
H,0,-1.0749636937,1.0909192278,4.6852366324
H,0,-1.7583746742,-0.495663308,4.2737609556

B3LYP/6-31G*
E(RB3LYP) = -337.700062441

Zero-point correction= 0.202597 (Hartree/Particle)
Thermal correction to Energy= 0.213811
Thermal correction to Enthalpy= 0.214755
Thermal correction to Gibbs Free Energy= 0.166918
Sum of electronic and zero-point Energies= -337.497465
Sum of electronic and thermal Energies= -337.486251
Sum of electronic and thermal Enthalpies= -337.485307
Sum of electronic and thermal Free Energies= -337.533144

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.169	40.546	100.682

C,0,2.2228675669,0.5108998379,1.1989505078
C,0,2.6743042264,-0.6451554951,2.0635349911
C,0,1.9296119597,-1.0141686185,3.1562292753
O,0,0.7800033624,-0.3871373137,3.476693518
H,0,1.7065481652,1.2733096124,1.7853686495
B,0,3.6558189758,-0.0019070079,3.6776918498
C,0,3.6303529847,-1.6329985789,1.4314719993
H,0,1.5293749123,0.1495146074,0.4273165965
H,0,3.0780212348,0.9719203343,0.6959060603
H,0,2.9937124803,0.5684670545,4.5074533157
H,0,4.3302487634,-0.9188229979,4.06201604
H,0,4.2052509399,0.7732957517,2.9374642626
H,0,2.1422926885,-1.9333290314,3.7017876896
C,0,0.3341858408,-0.5400340543,4.8356296673
C,0,-1.0651010018,0.0371904188,4.9367965389
H,0,0.34502003,-1.607660492,5.0989861234

H,0,1.0366026258,-0.0171953649,5.4950915333
H,0,4.5644159133,-1.1397446825,1.1446908635
H,0,3.8747774092,-2.4590744018,2.1047888912
H,0,3.1775301757,-2.0524322912,0.522603775
H,0,-1.43406211,-0.0570742739,5.9636689128
H,0,-1.0648895294,1.0975984459,4.6660014348
H,0,-1.7541936141,-0.4904274589,4.2697175043

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194493	E(Thermal)=	0.206042
E(QCISD(T))=	-336.598592	E(Empiric)=	-0.162240
DE(Plus)=	-0.019896	DE(2DF)=	-0.327886
E(Delta-G3)=	-0.460703	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.374822	G3 Energy=	-337.363274
G3 Enthalpy=	-337.362330	G3 Free Energy=	-337.410851

6e-7 Complex
B3LYP/6-31G**
E(RB3LYP) = -337.716208278

Zero-point correction=	0.201806 (Hartree/Particle)
Thermal correction to Energy=	0.212913
Thermal correction to Enthalpy=	0.213857
Thermal correction to Gibbs Free Energy=	0.166442
Sum of electronic and zero-point Energies=	-337.514402
Sum of electronic and thermal Energies=	-337.503295
Sum of electronic and thermal Enthalpies=	-337.502351
Sum of electronic and thermal Free Energies=	-337.549767

E (Thermal)	CV	S	
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin Total 133.605
40.678	99.795		

O,0,2.4393235809,0.7775995176,1.5690041731
C,0,2.6432788026,-0.3936778481,2.1828067867
C,0,2.0944953599,-1.0073022844,3.2916200282
C,0,0.937327369,-0.4931741328,4.1303746214
C,0,1.3293496761,1.6691970685,1.8308609275
B,0,3.7891218643,-0.2754223347,4.0616014109
H,0,3.3871580637,-0.9490179696,1.6198080883
H,0,3.7892072841,0.9203850663,3.9686628964
H,0,3.4258998461,-0.6976312636,5.1297953356

H,0,4.727370985,-0.8613322898,3.5925331258
C,0,2.2901994203,-2.5154905761,3.3732243086
H,0,1.0395872834,2.0196445914,0.8360243308
H,0,0.4915922558,1.1093234921,2.2490303331
C,0,1.7404064999,2.8441305038,2.7046879875
H,0,0.9026674524,3.5462946193,2.7845892983
H,0,2.030117695,2.5262270645,3.7086614391
H,0,2.589285176,3.3703315581,2.2586842524
H,0,2.4302735539,-2.8272253059,4.4121475054
H,0,1.4044077957,-3.0305904109,2.9785076575
H,0,3.1605053764,-2.8492897018,2.8020974988
H,0,0.9600518137,-0.9893058429,5.1046163273
H,0,0.9824939559,0.579992021,4.3181239547
H,0,-0.0264321101,-0.731835542,3.6619157125

B3LYP/6-31G*
E(RB3LYP) = -337.686820394

Zero-point correction= 0.203375 (Hartree/Particle)
Thermal correction to Energy= 0.214390
Thermal correction to Enthalpy= 0.215334
Thermal correction to Gibbs Free Energy= 0.168120
Sum of electronic and zero-point Energies= -337.483446
Sum of electronic and thermal Energies= -337.472431
Sum of electronic and thermal Enthalpies= -337.471487
Sum of electronic and thermal Free Energies= -337.518701

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.532	40.333	99.370

O,0,2.4253367307,0.7772005114,1.5567773844
C,0,2.6384968317,-0.3859019036,2.1793238343
C,0,2.0921899607,-1.0046533079,3.2853102628
C,0,0.9287355152,-0.4993133581,4.1204742265
C,0,1.3238170177,1.6687652605,1.832759698
B,0,3.7859561861,-0.2698627163,4.0530108706
H,0,3.3904776936,-0.9356069698,1.6205695015
H,0,3.840009459,0.9197177978,3.8961010678
H,0,3.3864976627,-0.6117625796,5.1382320219
H,0,4.705711744,-0.9183285312,3.6307768298
C,0,2.3031748905,-2.5094821261,3.3757962443
H,0,1.0298446833,2.034148503,0.844036979
H,0,0.4824379361,1.1110473868,2.2478398172

C,0,1.7458349116,2.8306250149,2.7193748956
H,0,0.9137153694,3.5378464967,2.8165912159
H,0,2.0421804895,2.494701935,3.7161784464
H,0,2.5961415346,3.356441722,2.274375389
H,0,2.4684868125,-2.8112223068,4.4145371429
H,0,1.4128411946,-3.037112157,3.0061881133
H,0,3.1632638175,-2.8417605275,2.7876654674
H,0,0.9486330935,-0.9981504782,5.0940854653
H,0,0.9673402113,0.5742965414,4.3113901322
H,0,-0.0334347457,-0.7398042075,3.6479829937

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.195240	E(Thermal)=	0.206594
E(QCISD(T))=	-336.585127	E(Empiric)=	-0.162240
DE(Plus)=	-0.019712	DE(2DF)=	-0.329328
E(Delta-G3)=	-0.460799	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.361966	G3 Energy=	-337.350612
G3 Enthalpy=	-337.349668	G3 Free Energy=	-337.397562

6e-8 complex
B3LYP/6-31+G**
E(RB3LYP) = -337.727875484

Zero-point correction= 0.201026 (Hartree/Particle)
Thermal correction to Energy= 0.212325
Thermal correction to Enthalpy= 0.213270
Thermal correction to Gibbs Free Energy= 0.165143
Sum of electronic and ZPE= -337.526849
Sum of electronic and thermal Energies= -337.515550
Sum of electronic and thermal Enthalpies= -337.514606
Sum of electronic and thermal Free Energies= -337.562733

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	133.236	40.939	101.291

C,0,2.1071118717,0.4517579957,1.2305265316
C,0,2.7385453212,-0.6403923161,2.064124798
C,0,2.131255238,-1.0598316333,3.2218126437
O,0,0.9638515011,-0.5260551588,3.6412251084
H,0,1.5806014371,1.1785656084,1.8510645984
B,0,3.8032995886,0.1215963135,3.5896818546

C,0,3.7295739344,-1.5423561687,1.3610660199
H,0,1.3814503627,0.0123052681,0.533344892
H,0,2.8682473361,0.9736386856,0.6439861705
H,0,4.2079380047,0.9257219946,2.79152144
H,0,3.1655464462,0.6357755072,4.4703042258
H,0,4.5904915304,-0.7258937525,3.9133029782
H,0,2.4829074409,-1.9429026077,3.751382539
C,0,0.6085587704,-0.7562816914,5.0229117381
H,0,-0.0912404075,0.0479963833,5.2621539393
C,0,-0.0415600216,-2.1183905746,5.2283625416
H,0,1.5006798759,-0.6267637274,5.6454630812
H,0,-0.3478298279,-2.2259926124,6.2747663555
H,0,-0.9289509214,-2.2232126855,4.5968334702
H,0,0.6455629314,-2.9391581775,4.9974712516
H,0,4.5806495277,-0.9659489037,0.9860862647
H,0,4.112832274,-2.3268271044,2.0182021499
H,0,3.2404737857,-2.0207316424,0.5023874076

B3LYP/6-31G*
E(RB3LYP) = -337.698194978

Zero-point correction= 0.202680 (Hartree/Particle)
Thermal correction to Energy= 0.213864
Thermal correction to Enthalpy= 0.214809
Thermal correction to Gibbs Free Energy= 0.167025
Sum of electronic and ZPE= -337.495514
Sum of electronic and thermal Energies= -337.484331
Sum of electronic and thermal Enthalpies= -337.483386
Sum of electronic and thermal Free Energies= -337.531170

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.202	40.563	100.569

C,0,2.1075146482,0.4516302185,1.2342677505
C,0,2.7376592192,-0.6434723759,2.0658752707
C,0,2.1237968208,-1.0633292656,3.2194943429
O,0,0.9579094867,-0.5277610281,3.6331964213
H,0,1.5731746848,1.1713124171,1.857388771
B,0,3.801933928,0.1126623512,3.5855965944
C,0,3.7283788341,-1.5449697467,1.3622064538
H,0,1.3888366017,0.0164245736,0.5263902677
H,0,2.8702423781,0.9830853271,0.6574215979
H,0,4.1872005802,0.947692021,2.8080092325

H,0,3.1669086245,0.594688022,4.4886253614
H,0,4.6005870105,-0.7343016494,3.8833089542
H,0,2.474770722,-1.9447839832,3.7533266834
C,0,0.6063588962,-0.7474739186,5.0146843373
H,0,-0.1015383537,0.0522003214,5.2474714502
C,0,-0.0318937148,-2.1133047077,5.2316415049
H,0,1.4963376437,-0.6039234022,5.6375200711
H,0,-0.343396933,-2.216079407,6.2773335073
H,0,-0.9141238616,-2.2324575357,4.5945994355
H,0,0.6650944068,-2.9293149969,5.0103617314
H,0,4.5856224094,-0.9699958087,0.997897035
H,0,4.103521207,-2.3365199002,2.0165319617
H,0,3.245100761,-2.0153885261,0.4948332639

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194573	E(Thermal)=	0.206094
E(QCISD(T))=	-336.596902	E(Empiric)=	-0.162240
DE(Plus)=	-0.019758	DE(2DF)=	-0.328101
E(Delta-G3)=	-0.460556	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.372984	G3 Energy=	-337.361463
G3 Enthalpy=	-337.360519	G3 Free Energy=	-337.408987

For Anharmonic Corrections of 6e-8

Zero-point vibrational energy 532140.3 (Joules/Mol) 127.18458 (Kcal/Mol)
Warning -- explicit consideration of 16 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 84.72 137.01 198.41 229.90 289.46
(Kelvin) 296.08 343.88 361.11 405.50 414.97
448.23 505.56 575.21 638.74 705.63
806.63 1059.08 1168.99 1195.08 1201.62
1294.70 1373.02 1423.04 1481.84 1510.85
1554.77 1578.07 1615.65 1631.07 1697.69
1711.36 1718.17 1789.74 1813.85 1929.74
2008.02 2042.68 2071.87 2078.40 2087.09
2165.31 2175.90 2182.86 2186.15 2194.85
2199.44 2221.87 2403.75 3626.42 3723.00
3763.15 4373.74 4383.06 4398.09 4422.45
4473.04 4482.63 4483.87 4503.00 4521.44
4521.73 4550.57 4569.61

Zero-point correction=	0.202682 (Hartree/Particle)
Thermal correction to Energy=	0.213865
Thermal correction to Enthalpy=	0.214809

Thermal correction to Gibbs Free Energy= 0.167027
Sum of electronic and zero-point Energies= -337.495513
Sum of electronic and thermal Energies= -337.484330
Sum of electronic and thermal Enthalpies= -337.483386
Sum of electronic and thermal Free Energies= -337.531168

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.202	40.563	100.567

ZPE(harm) = 0.53214D+03 kJ/mol ZPE(anh)= 0.52281D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.69832D-90	0.90812D-89	
QZvib	0.11773D+04	0.35561D+03	
Energy	0.56150D+03	0.54961D+03	kJ/mol
Enthalpy	0.56398D+03	0.55209D+03	kJ/mol
Entropy	0.42077D+03	0.41883D+03	J/(mol K)
Sp.Heat(V)	0.16972D+03	0.15758D+03	J/(mol K)
Sp.Heat(P)	0.17803D+03	0.16589D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.69832D-90	0.90812D-89	
QZvib	0.11773D+04	0.35561D+03	
Energy	0.56150D+03	0.54961D+03	kJ/mol
Enthalpy	0.56398D+03	0.55209D+03	kJ/mol
Entropy	0.42077D+03	0.41883D+03	J/(mol K)
Sp.Heat(V)	0.16972D+03	0.15758D+03	J/(mol K)
Sp.Heat(P)	0.17803D+03	0.16589D+03	J/(mol K)

6e-9 Variational Transtino State

B3LYP/6-31+G**
E(RB3LYP) = -337.723536487

Zero-point correction= 0.200723 (Hartree/Particle)
Thermal correction to Energy= 0.210952
Thermal correction to Enthalpy= 0.211896
Thermal correction to Gibbs Free Energy= 0.166068
Sum of electronic and ZPE= -337.522813
Sum of electronic and thermal Energies= -337.512584
Sum of electronic and thermal Enthalpies= -337.511640

Sum of electronic and thermal Free Energies= -337.557469

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	132.374	37.899	96.454

O,0,0.8700354114,0.3608367349,2.3825621218
C,0,1.9220421047,-0.4909420368,2.4490389255
C,0,2.0863009004,-1.3500119841,3.5885563547
C,0,1.0179441389,-1.302204767,4.6761439071
C,0,0.970043872,1.4005284503,1.3925546463
B,0,3.2845775741,-0.1637884436,3.7088630345
H,0,2.3429346939,-0.7969875915,1.4888713086
H,0,4.380765857,-0.6076198213,3.5104382069
H,0,3.1229326396,0.5599344853,2.6803684106
H,0,3.0326084854,0.5988205391,4.5974344271
C,0,2.6123681232,-2.7549989475,3.3035216082
H,0,1.4299848982,-1.6808984428,5.6171587601
H,0,0.6566379831,-0.2871886256,4.848782205
H,0,0.1580472894,-1.9307150714,4.4077009777
H,0,1.1766528059,0.9451206535,0.4136692502
C,0,-0.3343033753,2.1740206874,1.3768747825
H,0,1.8179385538,2.0477456791,1.6571408618
H,0,3.1216867408,-3.1542969774,4.1868545803
H,0,1.7936724779,-3.4418489434,3.048488079
H,0,3.3348204755,-2.7621323836,2.4813455388
H,0,-0.2786826505,2.9791986182,0.6371956187
H,0,-1.1721261747,1.5208008244,1.1157420792
H,0,-0.5322068241,2.6180733639,2.3566603155

B3LYP/6-31G*
E(RB3LYP) = -337.692674451

Zero-point correction= 0.202257 (Hartree/Particle)
Thermal correction to Energy= 0.212433
Thermal correction to Enthalpy= 0.213377
Thermal correction to Gibbs Free Energy= 0.167617
Sum of electronic and ZPE= -337.490418
Sum of electronic and thermal Energies= -337.480241
Sum of electronic and thermal Enthalpies= -337.479297
Sum of electronic and thermal Free Energies= -337.525057

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 133.304 37.545 96.310

O,0,0.8725698537,0.3531058191,2.3757226024
C,0,1.9298917273,-0.4898953428,2.4439105069
C,0,2.0931917173,-1.3473674227,3.5899413734
C,0,1.0123420638,-1.296091078,4.6648979448
C,0,0.9715458911,1.3938572179,1.392194034
B,0,3.2825093311,-0.1656688215,3.7147253894
H,0,2.3481026621,-0.8025887776,1.4837239358
H,0,4.3835252112,-0.5968784472,3.5110217041
H,0,3.1125508309,0.5470935099,2.6694468518
H,0,3.0293119662,0.6134118688,4.589333869
C,0,2.6149496541,-2.7539920845,3.3083775333
H,0,1.4115967282,-1.672747043,5.6128859805
H,0,0.6511737391,-0.2792194843,4.8304252778
H,0,0.152723409,-1.9235010119,4.3905772857
H,0,1.1712178172,0.9454834652,0.4078342413
C,0,-0.3311047872,2.1710425384,1.390914045
H,0,1.8242590569,2.0380840125,1.6510555038
H,0,3.1197204962,-3.1553858391,4.1941041728
H,0,1.7969059978,-3.4412458481,3.0496852792
H,0,3.341419748,-2.7642978115,2.4887734847
H,0,-0.2825847288,2.9808797277,0.6552937944
H,0,-1.1720528948,1.5190264603,1.134893737
H,0,-0.5190894901,2.6083403924,2.376227453

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194166	E(Thermal)=	0.204662
E(QCISD(T))=	-336.591839	E(Empiric)=	-0.162240
DE(Plus)=	-0.020075	DE(2DF)=	-0.329233
E(Delta-G3)=	-0.459443	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.368664	G3 Energy=	-337.358167
G3 Enthalpy=	-337.357223	G3 Free Energy=	-337.403609

For Anharmonic Corrections of 6e-9

Zero-point vibrational energy 531025.4 (Joules/Mol)
126.91813 (Kcal/Mol)
Warning -- explicit consideration of 14 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 96.17 155.53 187.82 296.26 301.16
(Kelvin) 344.05 374.09 402.49 440.71 506.78
528.67 609.64 745.80 794.80 1026.90
1106.40 1189.79 1200.46 1242.56 1313.36

1418.41 1467.80 1512.79 1525.14 1549.59
1627.49 1639.73 1656.93 1698.02 1717.94
1745.92 1800.58 1847.68 1891.95 1957.15
2034.35 2064.98 2078.64 2090.91 2157.31
2175.56 2179.98 2193.24 2199.10 2203.65
2224.59 2236.39 3135.45 3678.86 3824.69
4340.61 4358.46 4369.37 4395.89 4410.52
4454.13 4462.79 4479.35 4490.59 4513.49
4523.09 4538.69

Zero-point correction= 0.202257 (Hartree/Particle)
Thermal correction to Energy= 0.212434
Thermal correction to Enthalpy= 0.213378
Thermal correction to Gibbs Free Energy= 0.167617
Sum of electronic and zero-point Energies= -337.490418
Sum of electronic and thermal Energies= -337.480241
Sum of electronic and thermal Enthalpies= -337.479297
Sum of electronic and thermal Free Energies= -337.525057

E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	133.304	37.546	96.311

ZPE(harm) = 0.53103D+03 kJ/mol ZPE(anh)= 0.52299D+03 kJ/mol
Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.38121D-90	0.11472D-88	
QZvib	0.40991D+03	0.48186D+03	
Energy	0.55774D+03	0.55023D+03	kJ/mol
Enthalpy	0.56022D+03	0.55271D+03	kJ/mol
Entropy	0.41128D+03	0.41438D+03	J/(mol K)
Sp.Heat(V)	0.15709D+03	0.16025D+03	J/(mol K)
Sp.Heat(P)	0.16541D+03	0.16856D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.38121D-90	0.11472D-88	
QZvib	0.40991D+03	0.48186D+03	
Energy	0.55774D+03	0.55023D+03	kJ/mol
Enthalpy	0.56022D+03	0.55271D+03	kJ/mol
Entropy	0.41128D+03	0.41438D+03	J/(mol K)
Sp.Heat(V)	0.15709D+03	0.16025D+03	J/(mol K)
Sp.Heat(P)	0.16541D+03	0.16856D+03	J/(mol K)

6e-10 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -337.723536487

Zero-point correction= 0.200723 (Hartree/Particle)
Thermal correction to Energy= 0.210952
Thermal correction to Enthalpy= 0.211896
Thermal correction to Gibbs Free Energy= 0.166068
Sum of electronic and ZPE= -337.522813
Sum of electronic and thermal Energies= -337.512584
Sum of electronic and thermal Enthalpies= -337.511640
Sum of electronic and thermal Free Energies= -337.557469

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	132.374	37.899	96.454

C,0,2.1471000279,0.5325529335,1.1767296808
C,0,2.7587372468,-0.5337004895,2.0797922149
C,0,1.9983357893,-0.9631111883,3.2203526884
O,0,0.7991958675,-0.3942939091,3.4945326808
H,0,1.6089769163,1.2909567186,1.7475633724
B,0,3.5662705093,0.058288236,3.4417416347
C,0,3.5115371176,-1.6248058164,1.3216620003
H,0,1.4470775259,0.0831057074,0.4594604924
H,0,2.9367801307,1.0328873268,0.6068469988
H,0,3.4350406829,1.2459659306,3.5243275212
H,0,2.881591486,-0.3562265194,4.4251527062
H,0,4.6076778247,-0.5057160831,3.6297772382
H,0,2.1366644975,-1.978287158,3.5985315152
C,0,0.2798202603,-0.6377714687,4.8143974519
C,0,-1.1093472602,-0.0356403657,4.9010552555
H,0,0.2579939953,-1.721496409,4.9970556003
H,0,0.9627289448,-0.179352001,5.5433067186
H,0,4.3751493613,-1.1968130347,0.8019336267
H,0,3.8892502877,-2.4026953857,1.9926182999
H,0,2.8687576352,-2.1016338658,0.568975395
H,0,-1.5221944629,-0.1990329352,5.901750257
H,0,-1.0763351126,1.0412604784,4.7125797528
H,0,-1.7803992712,-0.496000702,4.1698978983

B3LYP/6-31G*
E(RB3LYP) = -337.692674452

Zero-point correction= 0.202257 (Hartree/Particle)
Thermal correction to Energy= 0.212433
Thermal correction to Enthalpy= 0.213377
Thermal correction to Gibbs Free Energy= 0.167617
Sum of electronic and ZPE= -337.490418
Sum of electronic and thermal Energies= -337.480241
Sum of electronic and thermal Enthalpies= -337.479297
Sum of electronic and thermal Free Energies= -337.525057

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	133.304	37.545	96.310

C,0,2.1366255054,0.5275551228,1.1845151647
C,0,2.7647275446,-0.5320568496,2.0840187597
C,0,2.0034248368,-0.9678216659,3.2267547292
O,0,0.8012385958,-0.404559796,3.4926765694
H,0,1.5957403553,1.2811600609,1.7601823493
B,0,3.5668843437,0.062325243,3.436687008
C,0,3.5152361063,-1.620633357,1.321233237
H,0,1.4345813729,0.0738736806,0.470970165
H,0,2.9165588238,1.0365264052,0.607793798
H,0,3.4254669996,1.2479488424,3.538242266
H,0,2.8719493384,-0.3708640326,4.4159454784
H,0,4.607514265,-0.4996372905,3.639071343
H,0,2.1410923755,-1.9863484342,3.5986251453
C,0,0.2828265748,-0.6420043092,4.8099305818
C,0,-1.1009408505,-0.0262699777,4.8934561063
H,0,0.2510167848,-1.7253065125,4.9978575468
H,0,0.9689552107,-0.1906163634,5.5411169165
H,0,4.376102853,-1.1912147632,0.7968952088
H,0,3.898288657,-2.3987546986,1.9901232004
H,0,2.8719197582,-2.1007703426,0.5702022917
H,0,-1.520070177,-0.1827306784,5.8930451404
H,0,-1.0553095114,1.0499855354,4.7010968825
H,0,-1.7734197628,-0.4813458191,4.1596011119

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194166	E(Thermal)=	0.204662
E(QCISD(T))=	-336.591839	E(Empiric)=	-0.162240
DE(Plus)=	-0.020075	DE(2DF)=	-0.329233

E(Delta-G3)=	-0.459443	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.368664	G3 Energy=	-337.358167
G3 Enthalpy=	-337.357223	G3 Free Energy=	-337.403609

For Anharmonic Corrections of 6e-10

Zero-point vibrational energy 531025.3 (Joules/Mol) 126.91810 (Kcal/Mol)
Warning -- explicit consideration of 14 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 96.17 155.53 187.82 296.26 301.16
(Kelvin) 344.05 374.09 402.49 440.71 506.78
528.67 609.64 745.80 794.79 1026.90
1106.40 1189.79 1200.46 1242.56 1313.36
1418.41 1467.80 1512.78 1525.14 1549.58
1627.49 1639.73 1656.93 1698.01 1717.94
1745.92 1800.58 1847.68 1891.95 1957.15
2034.35 2064.98 2078.64 2090.91 2157.31
2175.56 2179.98 2193.24 2199.10 2203.65
2224.59 2236.38 3135.42 3678.87 3824.70
4340.61 4358.46 4369.37 4395.89 4410.52
4454.13 4462.79 4479.35 4490.59 4513.49
4523.09 4538.69

Zero-point correction= 0.202257 (Hartree/Particle)
Thermal correction to Energy= 0.212434
Thermal correction to Enthalpy= 0.213378
Thermal correction to Gibbs Free Energy= 0.167617
Sum of electronic and zero-point Energies= -337.490418
Sum of electronic and thermal Energies= -337.480241
Sum of electronic and thermal Enthalpies= -337.479297
Sum of electronic and thermal Free Energies= -337.525057

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	133.304	37.546	96.311

ZPE(harm) = 0.53103D+03 kJ/mol ZPE(anh)= 0.52298D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.38122D-90	0.11455D-88	
QZvib	0.40990D+03	0.48015D+03	
Energy	0.55774D+03	0.55022D+03	kJ/mol
Enthalpy	0.56022D+03	0.55270D+03	kJ/mol
Entropy	0.41128D+03	0.41434D+03	J/(mol K)

Sp.Heat(V)	0.15709D+03	0.16025D+03	J/(mol K)
Sp.Heat(P)	0.16541D+03	0.16857D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.38122D-90	0.11455D-88	
QZvib	0.40990D+03	0.48015D+03	
Energy	0.55774D+03	0.55022D+03	kJ/mol
Enthalpy	0.56022D+03	0.55270D+03	kJ/mol
Entropy	0.41128D+03	0.41434D+03	J/(mol K)
Sp.Heat(V)	0.15709D+03	0.16025D+03	J/(mol K)
Sp.Heat(P)	0.16541D+03	0.16857D+03	J/(mol K)

6e-11 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -337.711883147

Zero-point correction= 0.200822 (Hartree/Particle)
Thermal correction to Energy= 0.211079
Thermal correction to Enthalpy= 0.212023
Thermal correction to Gibbs Free Energy= 0.165851
Sum of electronic and ZPE= -337.511061
Sum of electronic and thermal Energies= -337.500804
Sum of electronic and thermal Enthalpies= -337.499860
Sum of electronic and thermal Free Energies= -337.546032

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	132.454	38.068	97.178

O,0,1.7674275916,1.1174165072,2.4126186467
C,0,2.1005190275,-0.2213784035,2.5437219026
C,0,2.1589974734,-0.8774861315,3.8040783644
C,0,1.8231789797,-0.1123558554,5.0763627931
C,0,0.3482987248,1.3662194391,2.3552804426
B,0,3.7621208493,-0.5462876695,3.2094339421
H,0,1.945105888,-0.8304354254,1.6517284503
H,0,4.2907708621,-1.5686938199,2.8844557877
H,0,3.663096664,0.0875047137,2.1454099352

H,0,4.2484421345,0.2512672228,3.9540598232
C,0,1.8395397178,-2.3658284754,3.8548028207
H,0,2.4083158566,-0.498366209,5.9168837359
H,0,2.0374317349,0.9530459022,4.9758024007
H,0,0.761055379,-0.2335708988,5.3306617053
H,0,0.2516275911,2.4293817652,2.5909850298
C,0,-0.2530527932,1.0657526224,0.9860621866
H,0,-0.1587686335,0.7957627444,3.1440850804
H,0,2.440009736,-2.8651665398,4.6221670606
H,0,0.7809327485,-2.5251241937,4.1018196811
H,0,2.0480036418,-2.8603914953,2.9016700996
H,0,-1.3089168539,1.3587508609,0.9753565059
H,0,0.2682889666,1.6277875033,0.2053635651
H,0,-0.2036452867,0.0003058357,0.7387860403

B3LYP/6-31G*
E(RB3LYP) = -337.681253931

Zero-point correction= 0.202301 (Hartree/Particle)
Thermal correction to Energy= 0.212517
Thermal correction to Enthalpy= 0.213461
Thermal correction to Gibbs Free Energy= 0.167334
Sum of electronic and ZPE= -337.478953
Sum of electronic and thermal Energies= -337.468737
Sum of electronic and thermal Enthalpies= -337.467793
Sum of electronic and thermal Free Energies= -337.513920

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	133.356	37.731	97.082

O,0,1.7643805156,1.1182728007,2.4220063933
C,0,2.0970591593,-0.2193347692,2.5458867862
C,0,2.1691475018,-0.8796590245,3.8076711251
C,0,1.826792834,-0.1121339708,5.0767867535
C,0,0.3475933221,1.361763281,2.3599940374
B,0,3.7573138595,-0.5486493039,3.2175687147
H,0,1.9246307093,-0.828311335,1.6557738051
H,0,4.2947890107,-1.5643638218,2.8827278248
H,0,3.6341648588,0.0693259649,2.13844755
H,0,4.2537251883,0.2695703058,3.9340999636
C,0,1.8401144474,-2.3658418772,3.8554607856
H,0,2.4132588962,-0.4893388164,5.9211269262
H,0,2.0343034106,0.9545171088,4.9700791938

H,0,0.764678838,-0.2366764815,5.332761819
H,0,0.2440914187,2.4233850082,2.6016266271
C,0,-0.2436966525,1.0681934515,0.9848883081
H,0,-0.1651869373,0.7861160491,3.1418812293
H,0,2.438328075,-2.8715340892,4.621268487
H,0,0.7805778499,-2.5234128694,4.1026159522
H,0,2.0454255935,-2.8603292727,2.9005972693
H,0,-1.3002425048,1.3594362941,0.9636389016
H,0,0.2863095407,1.6336729815,0.2118676043
H,0,-0.1887789348,0.0034423859,0.7328199427

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194209	E(Thermal)=	0.204746
E(QCISD(T))=	-336.581547	E(Empiric)=	-0.162240
DE(Plus)=	-0.020041	DE(2DF)=	-0.329235
E(Delta-G3)=	-0.459486	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.358340	G3 Energy=	-337.347803
G3 Enthalpy=	-337.346858 3	Free Energy=	-337.393615

For Anharmonic Corrections 6e-11

Zero-point vibrational energy 531144.9 (Joules/Mol) 126.94667 (Kcal/Mol)

Warning -- explicit consideration of 14 degrees of freedom as vibrations may cause significant error

Vibrational temperatures: 63.86 122.64 201.73 313.57 326.80
(Kelvin) 337.91 362.44 403.87 492.35 513.31
541.02 619.37 679.28 838.61 979.09
1119.17 1162.00 1175.93 1213.54 1298.95
1416.90 1451.83 1491.34 1531.13 1533.75
1604.64 1613.52 1632.83 1673.16 1689.74
1741.28 1759.70 1816.44 1926.40 1971.47
2034.86 2065.18 2072.34 2088.27 2139.26
2172.32 2184.98 2188.16 2193.93 2201.69
2215.64 2235.98 3350.85 3706.61 3857.00
4356.92 4363.86 4385.03 4396.78 4456.85
4463.39 4473.79 4487.49 4496.93 4499.22
4516.86 4540.17

Zero-point correction=	0.202302 (Hartree/Particle)
Thermal correction to Energy=	0.212518
Thermal correction to Enthalpy=	0.213462
Thermal correction to Gibbs Free Energy=	0.167336
Sum of electronic and zero-point Energies=	-337.478952
Sum of electronic and thermal Energies=	-337.468736

Sum of electronic and thermal Enthalpies= -337.467792
Sum of electronic and thermal Free Energies= -337.513918

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	133.357	37.730	97.081

ZPE(harm) = 0.53114D+03 kJ/mol ZPE(anh)= 0.52400D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.54258D-90	0.12916D-88	
QZvib	0.61223D+03	0.81526D+03	
Energy	0.55797D+03	0.55090D+03	kJ/mol
Enthalpy	0.56044D+03	0.55338D+03	kJ/mol
Entropy	0.41450D+03	0.41718D+03	J/(mol K)
Sp.Heat(V)	0.15786D+03	0.16003D+03	J/(mol K)
Sp.Heat(P)	0.16618D+03	0.16834D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.54258D-90	0.12916D-88	
QZvib	0.61223D+03	0.81526D+03	
Energy	0.55797D+03	0.55090D+03	kJ/mol
Enthalpy	0.56044D+03	0.55338D+03	kJ/mol
Entropy	0.41450D+03	0.41718D+03	J/(mol K)
Sp.Heat(V)	0.15786D+03	0.16003D+03	J/(mol K)
Sp.Heat(P)	0.16618D+03	0.16834D+03	J/(mol K)

6e-12 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -337.721311980

Zero-point correction= 0.200848 (Hartree/Particle)
Thermal correction to Energy= 0.211043
Thermal correction to Enthalpy= 0.211988
Thermal correction to Gibbs Free Energy= 0.165980
Sum of electronic and ZPE= -337.520463
Sum of electronic and thermal Energies= -337.510269
Sum of electronic and thermal Enthalpies= -337.509324
Sum of electronic and thermal Free Energies= -337.555332

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	132.432	37.863	96.831

C,0,2.1162115977,0.4548842925,1.1887838597
C,0,2.8468371666,-0.5639529989,2.0573227746
C,0,2.1949120588,-1.0140840926,3.2560429098
O,0,0.9912717815,-0.4966776023,3.6054830963
H,0,1.5823177077,1.1937663176,1.7883341462
B,0,3.7190729124,0.090871202,3.3499255908
C,0,3.600612698,-1.6254118373,1.2592653049
H,0,1.3902834606,-0.041382118,0.5304984657
H,0,2.8349029163,0.9857949834,0.5560019449
H,0,3.5317510727,1.2711122411,3.4278837723
H,0,3.1282166287,-0.3455955963,4.3843445673
H,0,4.7987325449,-0.4175875045,3.4672297629
H,0,2.4207709456,-2.0132280364,3.6294778795
C,0,0.5451754999,-0.7414874487,4.9550237227
H,0,-0.2533823165,-0.0127109926,5.1116379947
C,0,0.0289429025,-2.1597531219,5.1654489556
H,0,1.3672201449,-0.5021062518,5.6434126763
H,0,-0.3570975724,-2.2600265713,6.1856981194
H,0,-0.7834524747,-2.3821976672,4.4670654908
H,0,0.8141290469,-2.9113807572,5.0361214167
H,0,4.3992486074,-1.1605399289,0.6716904369
H,0,4.0688788092,-2.3706683599,1.9099916958
H,0,2.9317688613,-2.1487131508,0.5621484162

B3LYP/6-31G*
E(RB3LYP) = -337.690695132

Zero-point correction= 0.202390 (Hartree/Particle)
Thermal correction to Energy= 0.212525
Thermal correction to Enthalpy= 0.213470
Thermal correction to Gibbs Free Energy= 0.167592
Sum of electronic and ZPE= -337.488305
Sum of electronic and thermal Energies= -337.478170
Sum of electronic and thermal Enthalpies= -337.477226
Sum of electronic and thermal Free Energies= -337.523103

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	133.362	37.509	96.556

C,0,2.1105542576,0.4500328589,1.1952655264
C,0,2.8545713177,-0.5616332233,2.0607588729
C,0,2.2022562396,-1.0135652539,3.2635389628
O,0,0.9960743558,-0.4988407415,3.6043478911
H,0,1.5784081516,1.1879999644,1.7985174118
B,0,3.7239331471,0.0955874922,3.3417470666
C,0,3.6018568154,-1.6246951863,1.2598151168
H,0,1.3802494665,-0.0494863107,0.5433267399
H,0,2.8198821526,0.9843424207,0.553811928
H,0,3.5320959559,1.2744352079,3.4364043873
H,0,3.1224875056,-0.3551337038,4.3746022206
H,0,4.8020389083,-0.4140904725,3.474289488
H,0,2.4247615398,-2.0160908985,3.6325075406
C,0,0.549323008,-0.7392331262,4.9509444644
H,0,-0.2470818296,-0.007483457,5.1082781895
C,0,0.027187791,-2.1555157152,5.1603299014
H,0,1.370374525,-0.5035948441,5.6425860834
H,0,-0.3649622621,-2.2575050837,6.1784772034
H,0,-0.7811540754,-2.3748989382,4.4555838766
H,0,0.8119096978,-2.9088824256,5.0321696083
H,0,4.3982994778,-1.1621254292,0.666373833
H,0,4.0735151067,-2.3700473165,1.9092469584
H,0,2.9307437472,-2.1506508178,0.565909729

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194294	E(Thermal)=	0.204750
E(QCISD(T))=	-336.589989	E(Empiric)=	-0.162240
DE(Plus)=	-0.019915	DE(2DF)=	-0.329370
E(Delta-G3)=	-0.459324	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.366542	G3 Energy=	-337.356087
G3 Enthalpy=	-337.355142	G3 Free Energy=	-337.401645

For Anharmonic Corrections of 6e-12

Zero-point vibrational energy 531375.9 (Joules/Mol) 127.00189 (Kcal/Mol)
Warning -- explicit consideration of 14 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 68.08 140.17 236.15 283.38 307.13
(Kelvin) 340.50 360.63 433.50 477.60 507.66
541.46 640.43 730.08 800.17 1021.53
1108.35 1170.06 1191.85 1244.61 1290.02
1416.95 1459.88 1503.93 1524.80 1539.11
1611.58 1632.23 1640.37 1691.71 1704.96

1743.03 1799.66 1851.51 1927.86 1965.88
2040.12 2064.34 2077.13 2087.02 2143.35
2175.83 2187.84 2191.39 2192.87 2203.77
2215.11 2233.27 3130.47 3680.19 3827.33
4357.79 4369.49 4372.24 4400.29 4453.78
4462.28 4482.32 4487.44 4504.14 4511.27
4521.17 4540.48

Zero-point correction= 0.202390 (Hartree/Particle)
Thermal correction to Energy= 0.212526
Thermal correction to Enthalpy= 0.213470
Thermal correction to Gibbs Free Energy= 0.167593
Sum of electronic and zero-point Energies= -337.488305
Sum of electronic and thermal Energies= -337.478169
Sum of electronic and thermal Enthalpies= -337.477225
Sum of electronic and thermal Free Energies= -337.523102

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	133.362	37.509	96.556

ZPE(harm) = 0.53138D+03 kJ/mol ZPE(anh)= 0.52303D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.39579D-90	0.34723D-88	
QZvib	0.49022D+03	0.14860D+04	
Energy	0.55799D+03	0.55088D+03	kJ/mol
Enthalpy	0.56047D+03	0.55336D+03	kJ/mol
Entropy	0.41231D+03	0.42568D+03	J/(mol K)
Sp.Heat(V)	0.15694D+03	0.16115D+03	J/(mol K)
Sp.Heat(P)	0.16525D+03	0.16947D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.39579D-90	0.34723D-88	
QZvib	0.49022D+03	0.14860D+04	
Energy	0.55799D+03	0.55088D+03	kJ/mol
Enthalpy	0.56047D+03	0.55336D+03	kJ/mol
Entropy	0.41231D+03	0.42568D+03	J/(mol K)
Sp.Heat(V)	0.15694D+03	0.16115D+03	J/(mol K)
Sp.Heat(P)	0.16525D+03	0.16947D+03	J/(mol K)

6e-13 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -337.722767252

Zero-point correction= 0.200641 (Hartree/Particle)
Thermal correction to Energy= 0.210850
Thermal correction to Enthalpy= 0.211794
Thermal correction to Gibbs Free Energy= 0.166091
Sum of electronic and ZPE= -337.522126
Sum of electronic and thermal Energies= -337.511917
Sum of electronic and thermal Enthalpies= -337.510973
Sum of electronic and thermal Free Energies= -337.556676

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	132.311	38.106	96.192

O,0,0.7685352136,0.3271207885,2.340073991
C,0,1.9274212889,-0.433673505,2.5084466911
C,0,1.9920715584,-1.2905615123,3.6441808031
C,0,0.8857162654,-1.2403530367,4.6756948477
C,0,0.9483911675,1.4849805275,1.5219077217
B,0,3.1374445585,0.1835359326,3.552454272
H,0,2.3563214793,-0.795972936,1.5724357063
H,0,4.2258915007,0.0053726871,3.0856558227
H,0,2.7489503672,1.2426469558,3.9546076632
H,0,3.1189459512,-0.5211184151,4.5792081811
C,0,2.7299484391,-2.606525519,3.5081659012
H,0,1.2114883397,-1.6725798455,5.6265215311
H,0,0.5398116124,-0.2192707053,4.8375004732
H,0,0.0365679924,-1.8236983598,4.2997058609
H,0,1.3392607635,1.1799823575,0.5381512495
C,0,-0.3934526642,2.1809063984,1.3741821278
H,0,1.6910803605,2.1468603402,1.9878795409
H,0,3.1265848359,-2.9442792612,4.4707343152
H,0,2.0281560872,-3.3647716583,3.1401832343
H,0,3.5569206502,-2.5318264723,2.7979709908
H,0,-0.2866481647,3.0725536467,0.7472518134
H,0,-1.1285303651,1.5166650902,0.9090109449
H,0,-0.7780092375,2.4903945018,2.3509733168

B3LYP/6-31G*
E(RB3LYP) = -337.691128729

Zero-point correction= 0.202165 (Hartree/Particle)
Thermal correction to Energy= 0.212299
Thermal correction to Enthalpy= 0.213243
Thermal correction to Gibbs Free Energy= 0.167673
Sum of electronic and ZPE= -337.488964
Sum of electronic and thermal Energies= -337.478830
Sum of electronic and thermal Enthalpies= -337.477886
Sum of electronic and thermal Free Energies= -337.523456

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	133.220	37.715	95.911

O,0,0.7737465497,0.3167674025,2.3281962047
C,0,1.9386000048,-0.4327686617,2.4994864829
C,0,1.9990954329,-1.2858435195,3.6433774112
C,0,0.8819940289,-1.2249436987,4.6634959315
C,0,0.9518267679,1.48355398,1.5301070004
B,0,3.1405354969,0.1864607093,3.531758138
H,0,2.361370086,-0.8096894329,1.5652995731
H,0,4.2358478949,-0.0059039037,3.0855466341
H,0,2.7608919511,1.2452316603,3.9458444342
H,0,3.1075094416,-0.5226703035,4.5639034792
C,0,2.7286939529,-2.6073073734,3.5160324892
H,0,1.194589003,-1.6467870675,5.6240933074
H,0,0.5357793724,-0.2010204153,4.8084225028
H,0,0.0359501023,-1.8119545121,4.2847664376
H,0,1.348982583,1.2001577913,0.5414610173
C,0,-0.3961138185,2.1702148203,1.3890050493
H,0,1.6886843343,2.1468959123,2.0044472413
H,0,3.1139332227,-2.9491592615,4.4824852115
H,0,2.0260766584,-3.3620639894,3.1409097978
H,0,3.5636085692,-2.538048748,2.8135902064
H,0,-0.3001296175,3.0726324585,0.7753096582
H,0,-1.1235243199,1.5033728335,0.9144690709
H,0,-0.785079697,2.459261319,2.3708897209

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194079	E(Thermal)=	0.204537
E(QCISD(T))=	-336.590744	E(Empiric)=	-0.162240
DE(Plus)=	-0.020899	DE(2DF)=	-0.328054
E(Delta-G3)=	-0.459743	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.367602	G3 Energy=	-337.357144
G3 Enthalpy=	-337.356199	G3 Free Energy=	-337.402399

For Anharmonic Correction Of 6e-13

Zero-point vibrational energy 530785.6 (Joules/Mol) 126.86081 (Kcal/Mol)
Warning -- explicit consideration of 15 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 106.08 153.64 193.40 283.10 303.49
(Kelvin) 334.04 370.61 438.16 464.00 501.43
535.93 721.87 746.15 827.73 874.25
1066.20 1180.74 1199.59 1219.02 1312.81
1395.09 1463.60 1478.12 1514.72 1558.78
1581.43 1636.96 1658.45 1669.61 1700.32
1718.86 1728.00 1820.51 1885.94 1958.06
2038.23 2063.66 2079.66 2083.20 2145.21
2169.04 2172.63 2180.18 2199.54 2203.96
2221.22 2242.49 3325.13 3683.80 3830.41
4308.54 4384.50 4390.27 4400.89 4401.44
4472.98 4482.94 4490.00 4503.46 4508.74
4525.63 4569.14

Zero-point correction= 0.202166 (Hartree/Particle)
Thermal correction to Energy= 0.212299
Thermal correction to Enthalpy= 0.213244
Thermal correction to Gibbs Free Energy= 0.167673
Sum of electronic and zero-point Energies= -337.488963
Sum of electronic and thermal Energies= -337.478829
Sum of electronic and thermal Enthalpies= -337.477885
Sum of electronic and thermal Free Energies= -337.523456

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	133.220	37.715	95.912

ZPE(harm) = 0.53079D+03 kJ/mol ZPE(anh)= 0.52254D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.36728D-90	0.17282D-88	
QZvib	0.35851D+03	0.60575D+03	
Energy	0.55739D+03	0.54946D+03	kJ/mol
Enthalpy	0.55987D+03	0.55194D+03	kJ/mol
Entropy	0.40961D+03	0.41503D+03	J/(mol K)
Sp.Heat(V)	0.15780D+03	0.15990D+03	J/(mol K)
Sp.Heat(P)	0.16611D+03	0.16821D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.36728D-90	0.17282D-88	
QZvib	0.35851D+03	0.60575D+03	
Energy	0.55739D+03	0.54946D+03	kJ/mol
Enthalpy	0.55987D+03	0.55194D+03	kJ/mol
Entropy	0.40961D+03	0.41503D+03	J/(mol K)
Sp.Heat(V)	0.15780D+03	0.15990D+03	J/(mol K)
Sp.Heat(P)	0.16611D+03	0.16821D+03	J/(mol K)

6e-15 Transition State

B3LYP/6-31G**
E(RB3LYP) = -337.720636808

Zero-point correction= 0.200807 (Hartree/Particle)
Thermal correction to Energy= 0.210954
Thermal correction to Enthalpy= 0.211899
Thermal correction to Gibbs Free Energy= 0.166185
Sum of electronic and zero-point Energies= -337.519830
Sum of electronic and thermal Energies= -337.509682
Sum of electronic and thermal Enthalpies= -337.508738
Sum of electronic and thermal Free Energies= -337.554452

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	132.376	38.066	96.212

C,0,2.197849,0.581752,1.303077
C,0,2.825318,-0.573997,2.051471
C,0,2.166976,-1.105745,3.197021
O,0,0.894429,-0.607007,3.487261
H,0,1.730304,1.290698,1.986507
B,0,3.520414,-0.207609,3.749289
C,0,3.722133,-1.492238,1.247509
H,0,1.412795,0.183475,0.649043
H,0,2.936695,1.099999,0.684645
H,0,4.03527,0.328035,2.751659
H,0,3.095665,0.731269,4.35947
H,0,4.366322,-0.944831,4.168714
H,0,2.293867,-2.1693,3.395773
C,0,0.499892,-0.668267,4.862716

H,0,-0.394405,-0.040227,4.919263
C,0,0.17949,-2.082139,5.342249
H,0,1.280754,-0.210117,5.483729
H,0,-0.209742,-2.043801,6.366095
H,0,-0.579458,-2.545945,4.70368
H,0,1.066051,-2.724283,5.352353
H,0,4.509942,-0.933093,0.733164
H,0,4.18956,-2.251276,1.879327
H,0,3.112759,-2.002094,0.491347

B3LYP/6-31G*
E(RB3LYP) = -337.690785607

Zero-point correction= 0.202325 (Hartree/Particle)
Thermal correction to Energy= 0.212387
Thermal correction to Enthalpy= 0.213332
Thermal correction to Gibbs Free Energy= 0.167796
Sum of electronic and zero-point Energies= -337.486957
Sum of electronic and thermal Energies= -337.476895
Sum of electronic and thermal Enthalpies= -337.475950
Sum of electronic and thermal Free Energies= -337.521486

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	133.275	37.672	95.837

C,0,2.1687682113,0.5502933845,1.2618122554
C,0,2.7634944035,-0.6146927633,2.0150487796
C,0,2.1547780014,-1.072743127,3.1824927984
O,0,0.9124593498,-0.5635194063,3.5171909471
H,0,1.6827443621,1.2542440177,1.938459279
B,0,3.5356941853,-0.1741867734,3.6611486826
C,0,3.7125372896,-1.5136566705,1.2591367695
H,0,1.4047305691,0.169795977,0.5706079753
H,0,2.9303834476,1.0738984797,0.6758612357
H,0,4.1329649025,0.5239849759,2.8622524446
H,0,3.0155390666,0.620639689,4.3998911441
H,0,4.3184639054,-0.9721675087,4.1039009359
H,0,2.3323749615,-2.098138825,3.5023977192
C,0,0.5379414024,-0.6636735647,4.895524792
H,0,-0.3343656575,-0.009449227,4.9882723042
C,0,0.1758763748,-2.0835460912,5.3231476861
H,0,1.3390602521,-0.2518570871,5.5223421151
H,0,-0.2015460958,-2.0745483623,6.3522794307

H,0,-0.6037018996,-2.4960726393,4.6738737442
H,0,1.0398776091,-2.7564301803,5.297432508
H,0,4.5334666597,-0.9405689378,0.8166946293
H,0,4.1376604411,-2.2894489968,1.9012739608
H,0,3.163678258,-2.0048973631,0.4443198632

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.194232	E(Thermal)=	0.204621
E(QCISD(T))=	-336.589078	E(Empiric)=	-0.162240
DE(Plus)=	-0.020843	DE(2DF)=	-0.328178
E(Delta-G3)=	-0.459516	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.365623	G3 Energy=	-337.355234
G3 Enthalpy=	-337.354290	G3 Free Energy=	-337.400454

6e-16 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -337.744522789

Zero-point correction= 0.202691 (Hartree/Particle)
Thermal correction to Energy= 0.213782
Thermal correction to Enthalpy= 0.214726
Thermal correction to Gibbs Free Energy= 0.166247
Sum of electronic and ZPE= -337.541831
Sum of electronic and thermal Energies= -337.530741
Sum of electronic and thermal Enthalpies= -337.529796
Sum of electronic and thermal Free Energies= -337.578276

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.150	39.569	102.033

O,0,1.0142473746,0.7098050126,2.7843362215
C,0,2.0499365771,-0.2872028841,2.7077940836
C,0,1.9445489393,-1.1483657138,4.0057293626
C,0,0.5334795647,-1.7398475691,4.1511893587
C,0,0.759368898,1.3679670838,1.553873174
B,0,3.4876966378,0.3142176994,2.4964707902
H,0,1.8173741941,-0.9725819896,1.8653175227
H,0,4.4101218393,-0.4005250594,2.2411298454
H,0,3.6825396914,1.4889612241,2.5976105777
H,0,2.1117708872,-0.469555615,4.8537415092
C,0,3.0030766882,-2.2629679894,4.0566078014

H,0,0.4428573311,-2.2781183942,5.101648544
H,0,-0.2282834708,-0.958492865,4.12012714
H,0,0.3282313536,-2.4522210318,3.3413776794
H,0,0.443488284,0.6302563252,0.7954516324
C,0,-0.326714657,2.4091402165,1.7707774014
H,0,1.6785946711,1.8493388903,1.178560797
H,0,2.836736421,-2.8966264248,4.9342925211
H,0,2.9423689779,-2.9061025556,3.1698430026
H,0,4.0246315622,-1.8762561828,4.1154567441
H,0,-0.5495354624,2.9272172441,0.8317575427
H,0,-1.2454180574,1.9375364979,2.1332746481
H,0,-0.0066302451,3.1504440805,2.5093810999

B3LYP/6-31G*
E(RB3LYP) = -337.713818851

Zero-point correction= 0.204288 (Hartree/Particle)
Thermal correction to Energy= 0.215316
Thermal correction to Enthalpy= 0.216260
Thermal correction to Gibbs Free Energy= 0.167990
Sum of electronic and ZPE= -337.509531
Sum of electronic and thermal Energies= -337.498503
Sum of electronic and thermal Enthalpies= -337.497559
Sum of electronic and thermal Free Energies= -337.545829

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.113	39.266	101.593

O,0,1.0173794814,0.7070939869,2.7811680723
C,0,2.0491086906,-0.2891596093,2.6992174186
C,0,1.9458408194,-1.1459895019,4.0007038731
C,0,0.5324696577,-1.7296150966,4.1462400037
C,0,0.7563219904,1.3544059995,1.5507800167
B,0,3.4878648308,0.3182781149,2.5084071519
H,0,1.8184449582,-0.9751749992,1.8577917198
H,0,4.4110227082,-0.3823487767,2.2135796449
H,0,3.6855689668,1.4864863854,2.6736873746
H,0,2.1154678595,-0.464238736,4.8461809587
C,0,3.0013598935,-2.2618811899,4.0532830439
H,0,0.4317845516,-2.2560406014,5.1029304701
H,0,-0.2227764535,-0.9424155172,4.0988166476
H,0,0.3275926156,-2.4505952729,3.3434760416
H,0,0.4307485869,0.6168979152,0.7952472

C,0,-0.3225897275,2.4016633992,1.7749186388
H,0,1.6737565237,1.8299571455,1.1603584397
H,0,2.8395944336,-2.8911930891,4.9357959537
H,0,2.9353915377,-2.9098536835,3.1699278362
H,0,4.0244018488,-1.8753860864,4.1042891955
H,0,-0.5591557081,2.9169258589,0.8373806301
H,0,-1.2365810771,1.9337090707,2.1551682089
H,0,0.0114710117,3.1444942839,2.5064004596

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.196116	E(Thermal)=	0.207462
E(QCISD(T))=	-336.614291	E(Empiric)=	-0.162240
DE(Plus)=	-0.020011	DE(2DF)=	-0.326496
E(Delta-G3)=	-0.459794	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.386716	G3 Energy=	-337.375370
G3 Enthalpy=	-337.374426	G3 Free Energy=	-337.423355

6e-17 Product
B3LYP/6-31+G**
E(RB3LYP) = -337.741757301

Zero-point correction= 0.202756 (Hartree/Particle)
Thermal correction to Energy= 0.213807
Thermal correction to Enthalpy= 0.214751
Thermal correction to Gibbs Free Energy= 0.166192
Sum of electronic and ZPE= -337.539001
Sum of electronic and thermal Energies= -337.527951
Sum of electronic and thermal Enthalpies= -337.527007
Sum of electronic and thermal Free Energies= -337.575566

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.166	39.625	102.201

C,0,1.5812424907,-0.3234411224,1.0208384994
C,0,2.8394342205,-0.2767218632,1.9025310258
C,0,2.5273406289,-0.8093875169,3.3370012374
O,0,1.4391764069,-0.0092714874,3.8412376707
H,0,0.7515074771,0.2106485621,1.4873992754
B,0,3.7926310592,-0.8115774493,4.2706337674
C,0,3.9941825255,-1.0378151835,1.2302096656
H,0,1.2685953234,-1.3617425035,0.848998808

H,0,1.7843935347,0.1306616669,0.0442066008
H,0,3.131827223,0.7771057272,2.011214655
H,0,3.8659912634,-0.0819712951,5.2140180602
H,0,4.7069045162,-1.5457745562,4.0424553671
H,0,2.1839780109,-1.8544989174,3.2000570033
C,0,0.8212454965,-0.4954332208,5.0266719501
H,0,0.3252574831,0.3721488663,5.4750090078
C,0,-0.2013691207,-1.6030171387,4.7689456267
H,0,1.5850061945,-0.8365407694,5.7447495172
H,0,-0.6836297471,-1.8945510802,5.7093336896
H,0,-0.9756098459,-1.2550808116,4.0779886724
H,0,0.2604738398,-2.4989392709,4.3409556628
H,0,4.1179072215,-0.6924247282,0.1982066819
H,0,4.9501300085,-0.8995721866,1.7433741431
H,0,3.7892957891,-2.1150487211,1.1941694123

B3LYP/6-31G*
E(RB3LYP) = -337.711355016

Zero-point correction= 0.204348 (Hartree/Particle)
Thermal correction to Energy= 0.215326
Thermal correction to Enthalpy= 0.216270
Thermal correction to Gibbs Free Energy= 0.167961
Sum of electronic and ZPE= -337.507007
Sum of electronic and thermal Energies= -337.496029
Sum of electronic and thermal Enthalpies= -337.495085
Sum of electronic and thermal Free Energies= -337.543394

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.119	39.308	101.675

C,0,1.5758194219,-0.3227216514,1.0352331563
C,0,2.8387396425,-0.2803488349,1.9087916896
C,0,2.5264470655,-0.8144089555,3.3432118238
O,0,1.4464041418,-0.0080171501,3.845619648
H,0,0.7494247385,0.2040780937,1.5164300597
B,0,3.7998905203,-0.7996189533,4.266986908
C,0,3.988724075,-1.0434662922,1.2330309271
H,0,1.2639838079,-1.3605325297,0.8565850889
H,0,1.7685384235,0.1410543273,0.060391996
H,0,3.1339668825,0.7727526826,2.0189053786
H,0,3.8982489226,-0.0209414229,5.1695731236
H,0,4.6995135479,-1.5626541448,4.0702627391

H,0,2.1832491489,-1.858933418,3.2080107978
C,0,0.8243385746,-0.4995434836,5.0220401828
H,0,0.3268949792,0.3649933083,5.4763294927
C,0,-0.1991821827,-1.6029982182,4.7519605223
H,0,1.5828065082,-0.8484814249,5.7436415537
H,0,-0.6927187618,-1.900236379,5.6850621728
H,0,-0.9645180934,-1.2486545781,4.0535427398
H,0,0.2656075864,-2.4970159716,4.3216319965
H,0,4.1162780986,-0.6940718619,0.2021288563
H,0,4.9454024253,-0.9126613676,1.7487216402
H,0,3.7780525266,-2.1198167743,1.1921135062

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.196175	E(Thermal)=	0.207473
E(QCISD(T))=	-336.612067	E(Empiric)=	-0.162240
DE(Plus)=	-0.019821	DE(2DF)=	-0.326664
E(Delta-G3)=	-0.459746	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.384365	G3 Energy=	-337.373066
G3 Enthalpy=	-337.372122	G3 Free Energy=	-337.421085

6e-18 Product
B3LYP/6-31+G**
E(RB3LYP) = -337.744522792

Zero-point correction= 0.202691 (Hartree/Particle)
Thermal correction to Energy= 0.213782
Thermal correction to Enthalpy= 0.214726
Thermal correction to Gibbs Free Energy= 0.166247
Sum of electronic and ZPE= -337.541831
Sum of electronic and thermal Energies= -337.530741
Sum of electronic and thermal Enthalpies= -337.529796
Sum of electronic and thermal Free Energies= -337.578276

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.150	39.569	102.033

O,0,1.6040717407,1.1171482477,2.4058106156
C,0,2.5019932787,0.0117286929,2.6163301488
C,0,1.8474887967,-0.9016069264,3.7002112405
C,0,0.4367396122,-1.3313690079,3.2675256575
C,0,1.8825308225,1.8675308703,1.2346704987

B,0,3.962744418,0.4517967084,2.9985088934
H,0,2.5387016988,-0.594195102,1.6862177335
H,0,4.8471133036,-0.3506360846,3.028817516
H,0,4.2091582647,1.5883446201,3.2737449244
H,0,1.7476932416,-0.2948544927,4.6111245294
C,0,2.7089502272,-2.1333048414,4.0261091797
C,0,0.8899058402,3.014893651,1.1401971601
H,0,2.9140308554,2.25818897,1.2654411005
H,0,1.8063961714,1.2148005203,0.3473443767
H,0,1.0776171294,3.6065159899,0.2376671104
H,0,-0.135499358,2.6345647554,1.0986706142
H,0,0.9775982643,3.6717966645,2.011006652
H,0,2.1739209157,-2.7907101795,4.7197127737
H,0,2.9247539966,-2.7149744363,3.1212618934
H,0,3.665760512,-1.872392471,4.4876532515
H,0,-0.0468294772,-1.9070438479,4.0650725899
H,0,-0.1870993228,-0.465879754,3.0361912247
H,0,0.4842560682,-1.9690725464,2.3750713155

B3LYP/6-31G*
E(RB3LYP) = -337.713818866

Zero-point correction= 0.204288 (Hartree/Particle)
Thermal correction to Energy= 0.215316
Thermal correction to Enthalpy= 0.216261
Thermal correction to Gibbs Free Energy= 0.167987
Sum of electronic and ZPE= -337.509531
Sum of electronic and thermal Energies= -337.498502
Sum of electronic and thermal Enthalpies= -337.497558
Sum of electronic and thermal Free Energies= -337.545831

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.113	39.265	101.599

O,0,1.6078248197,1.1142867179,2.4036321192
C,0,2.5040923022,0.010296646,2.6078797956
C,0,1.8507618224,-0.8990585207,3.696235256
C,0,0.4385190051,-1.320805185,3.2636761979
C,0,1.8797346103,1.8545402444,1.2292661579
B,0,3.9585807388,0.4550934318,3.0102754273
H,0,2.5420760251,-0.5966694056,1.6794915256
H,0,4.8600958961,-0.3305843084,3.0041207165
H,0,4.1827992557,1.5809096738,3.3470041991

H,0,1.7543545314,-0.2896823223,4.6060826791
C,0,2.7087417367,-2.1317630143,4.0223903142
C,0,0.8916623584,3.0067428062,1.1446085868
H,0,2.9146848034,2.2404407999,1.244874923
H,0,1.793637875,1.2029507986,0.3411527333
H,0,1.0662272372,3.5973523577,0.2384433451
H,0,-0.135661553,2.628577924,1.1211317962
H,0,0.9948019405,3.6636426167,2.0142694129
H,0,2.17702902,-2.7852552037,4.7232893827
H,0,2.9172177654,-2.7182440212,3.1184487341
H,0,3.6702258835,-1.870756754,4.4763320235
H,0,-0.0553004464,-1.8843827953,4.064327725
H,0,-0.1729474669,-0.4493615255,3.0207033877
H,0,0.4828388393,-1.9670009608,2.3767245613

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.196117	E(Thermal)=	0.207463
E(QCISD(T))=	-336.614292	E(Empiric)=	-0.162240
DE(Plus)=	-0.020010	DE(2DF)=	-0.326496
E(Delta-G3)=	-0.459795	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.386716	G3 Energy=	-337.375369
G3 Enthalpy=	-337.374425	G3 Free Energy=	-337.423356

6e-19 Product
B3LYP/6-31G**
E(RB3LYP) = -337.744522807

Zero-point correction= 0.202692 (Hartree/Particle)
Thermal correction to Energy= 0.213782
Thermal correction to Enthalpy= 0.214726
Thermal correction to Gibbs Free Energy= 0.166249
Sum of electronic and zero-point Energies= -337.541831
Sum of electronic and thermal Energies= -337.530741
Sum of electronic and thermal Enthalpies= -337.529796
Sum of electronic and thermal Free Energies= -337.578274

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	134.150	39.569	102.029

C,0,1.8107263845,-0.0124998547,0.9196799892
C,0,2.9139296626,-0.170097202,1.978109007
C,0,2.3330429827,-0.7793290207,3.2929002638

O,0,1.2563443846,0.0805959125,3.7098588872
H,0,0.9745074419,0.5746515607,1.3040865314
B,0,3.4320517054,-0.9919738433,4.3976636101
C,0,4.0840286294,-0.9955037802,1.4169293531
H,0,1.4282712443,-0.994459077,0.6116544963
H,0,2.207391972,0.4870023973,0.028348923
H,0,3.2836915507,0.8342329647,2.2279475711
H,0,3.4385691043,-0.3294648352,5.3922623044
H,0,4.2848475431,-1.8154702472,4.2509184986
H,0,1.9071869543,-1.7658585165,3.0118751053
C,0,0.4151161208,-0.4914794458,4.6983866694
C,0,-0.6578650339,0.5180590161,5.0728646255
H,0,-0.0427888661,-1.4170441078,4.3074144976
H,0,1.0038802286,-0.7692613676,5.5893226743
H,0,4.400588491,-0.5867725848,0.4513981352
H,0,4.9560868274,-0.9997710346,2.0773108792
H,0,3.7879173126,-2.0389022638,1.2517117937
H,0,-1.3277705784,0.0972710571,5.8304788105
H,0,-0.204794667,1.4286988861,5.4765716923
H,0,-1.2534003947,0.7903143866,4.195911682

B3LYP/6-31G*
E(RB3LYP) = -337.713818775

Zero-point correction= 0.204287 (Hartree/Particle)
Thermal correction to Energy= 0.215316
Thermal correction to Enthalpy= 0.216260
Thermal correction to Gibbs Free Energy= 0.167988
Sum of electronic and zero-point Energies= -337.509532
Sum of electronic and thermal Energies= -337.498503
Sum of electronic and thermal Enthalpies= -337.497559
Sum of electronic and thermal Free Energies= -337.545831

	E (Thermal)	CV	S	
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin	Total
135.113	39.266	101.597		

C,0,1.8003916937,-0.0266452126,0.9274635318
C,0,2.9098916472,-0.1818018572,1.9783655151
C,0,2.3299200563,-0.7851993655,3.2965840501
O,0,1.2598365449,0.0805570551,3.7080969777
H,0,0.9640250893,0.5525942821,1.3240677892
B,0,3.4400480969,-0.969428412,4.3962773499

C,0,4.0760266188,-1.011172799,1.4176993709
H,0,1.4209175435,-1.0097696663,0.6181433012
H,0,2.1863384924,0.4794948601,0.0345050618
H,0,3.2818629532,0.8231879925,2.2234993178
H,0,3.4790411274,-0.2514872136,5.3523839002
H,0,4.2745507625,-1.8185819528,4.2840921818
H,0,1.9058602727,-1.773986795,3.0241331257
C,0,0.4180910194,-0.4882733652,4.692440154
C,0,-0.6467611199,0.5306238297,5.0652672924
H,0,-0.0473417963,-1.4127921805,4.3059554129
H,0,1.0027223929,-0.7725792284,5.5855499452
H,0,4.3952236098,-0.6057540219,0.4508598267
H,0,4.9483012296,-1.0170244444,2.07932808
H,0,3.7764054801,-2.054364199,1.2548814512
H,0,-1.3252333463,0.1190104766,5.8207043188
H,0,-0.1841067816,1.4369950832,5.468884781
H,0,-1.2344525865,0.8093361343,4.1844232647

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.196115	E(Thermal)=	0.207462
E(QCISD(T))=	-336.614294	E(Empiric)=	-0.162240
DE(Plus)=	-0.020011	DE(2DF)=	-0.326495
E(Delta-G3)=	-0.459794	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.386718	G3 Energy=	-337.375371
G3 Enthalpy=	-337.374427	G3 Free Energy=	-337.423358

6e-20 Product
B3LYP/6-31+G**
E(RB3LYP) = -337.746270258

Zero-point correction= 0.203341 (Hartree/Particle)
Thermal correction to Energy= 0.213963
Thermal correction to Enthalpy= 0.214907
Thermal correction to Gibbs Free Energy= 0.168475
Sum of electronic and ZPE= -337.542929
Sum of electronic and thermal Energies= -337.532308
Sum of electronic and thermal Enthalpies= -337.531364
Sum of electronic and thermal Free Energies= -337.577795

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 134.263 39.219 97.724

O,0,0.5622816199,0.03553158,1.8104776029
C,0,1.5003046187,-1.0066971361,2.0493983926
C,0,1.9999408532,-1.0734440664,3.5178446955
C,0,0.8070691875,-1.3009939783,4.4667914296
C,0,1.1142081741,1.3332383762,1.8805989015
B,0,2.8665112365,0.192967825,3.8776298344
H,0,0.9686539831,-1.9326474151,1.7997080215
H,0,3.7904212919,0.491524436,3.1754139913
H,0,2.3571670891,-0.9033968264,1.3641154246
H,0,2.6975679534,0.8111490114,4.8895115121
C,0,2.9758558312,-2.2826728228,3.6017861872
H,0,1.1428250072,-1.375105688,5.5069912536
H,0,0.0879048081,-0.4787858813,4.404580135
H,0,0.2713685697,-2.2274422409,4.2187922669
H,0,1.9300028388,1.4423837982,1.1488390674
C,0,0.017737172,2.3571639149,1.6385717593
H,0,1.5610842501,1.5082527475,2.8873917074
H,0,3.382333888,-2.4044190061,4.6121042729
H,0,2.4435630992,-3.211239312,3.3545279562
H,0,3.8195784234,-2.1813549973,2.910433833
H,0,0.424878595,3.3716575939,1.6987715487
H,0,-0.4198451046,2.2155027603,0.6456438116
H,0,-0.7771373855,2.2546393274,2.3831443949

B3LYP/6-31G*
E(RB3LYP) = -337.715737711

Zero-point correction= 0.204915 (Hartree/Particle)
Thermal correction to Energy= 0.215443
Thermal correction to Enthalpy= 0.216387
Thermal correction to Gibbs Free Energy= 0.170188
Sum of electronic and ZPE= -337.510823
Sum of electronic and thermal Energies= -337.500295
Sum of electronic and thermal Enthalpies= -337.499351
Sum of electronic and thermal Free Energies= -337.545550

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 135.193 38.878 97.235

O,0,0.5642339122,0.0329153319,1.8145065619
C,0,1.5029502753,-1.0058222128,2.0475541137

C,0,2.0019644389,-1.0724198479,3.5164706463
C,0,0.8031314072,-1.2940075385,4.4579855238
C,0,1.120230427,1.3246746788,1.8789791831
B,0,2.8624917945,0.1995864941,3.8706581525
H,0,0.9737365014,-1.9335522373,1.7969613149
H,0,3.793509956,0.4926532044,3.1735386193
H,0,2.3602851651,-0.9026408748,1.3617190164
H,0,2.684519795,0.8291841829,4.8752186006
C,0,2.9729868461,-2.2831383987,3.60377558
H,0,1.1262429199,-1.347359315,5.5040224416
H,0,0.0782518656,-0.4784132087,4.3713702722
H,0,0.2769157732,-2.2294058922,4.2206903593
H,0,1.9285185727,1.4375296906,1.138247042
C,0,0.0205856262,2.3497854881,1.6553269199
H,0,1.585046601,1.5000567958,2.8797119919
H,0,3.3721782444,-2.4089156757,4.6171067672
H,0,2.4426931496,-3.2110988576,3.3478356634
H,0,3.8233399171,-2.1801424838,2.9197479898
H,0,0.4259660914,3.3656096924,1.7101576703
H,0,-0.4328418347,2.2070987936,0.6691492052
H,0,-0.7626614452,2.2436341904,2.4123343648

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.164055	E(Thermal)=	0.173379
E(QCISD(T))=	-310.081410	E(Empiric)=	-0.141960
DE(Plus)=	-0.018227	DE(2DF)=	-0.286352
E(Delta-G3)=	-0.413051	E(G3-Empiric)=	-0.141960
G3(0 K)=	-310.776945	G3 Energy=	-310.767621
G3 Enthalpy=	-310.766677	G3 Free Energy=	-310.812297

6e-21 Product
B3LYP/6-31+G**
E(RB3LYP) = -337.744685455

Zero-point correction= 0.202871 (Hartree/Particle)
Thermal correction to Energy= 0.214001
Thermal correction to Enthalpy= 0.214945
Thermal correction to Gibbs Free Energy= 0.166763
Sum of electronic and ZPE= -337.541815
Sum of electronic and thermal Energies= -337.530684
Sum of electronic and thermal Enthalpies= -337.529740
Sum of electronic and thermal Free Energies= -337.577922

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.288	39.882	101.408

C,0,2.4547193386,0.8176670876,1.5195762636
C,0,2.8259263396,-0.618596343,2.0222781444
C,0,2.2044077249,-0.8582617825,3.4050873033
O,0,0.7837284543,-0.7899186085,3.32540106
H,0,2.8152845909,1.6045802801,2.1938152305
B,0,4.3841409222,-0.4833853376,2.0914922575
C,0,2.3298009249,-1.6631417735,1.0013993433
H,0,1.3636967823,0.9008423086,1.4730438113
H,0,2.8551100603,1.010232966,0.5187392301
H,0,4.9361267353,-0.1567654133,3.1038856623
H,0,2.5683937645,-0.1004753053,4.1187536617
H,0,5.0393556925,-0.6147735319,1.0987302693
H,0,2.517467226,-1.8451526111,3.7811838252
C,0,0.1065134965,-0.8661183728,4.5753839811
H,0,-0.9089459802,-0.5096783184,4.3732484941
C,0,0.0544329197,-2.2753443631,5.1663595441
H,0,0.5689654982,-0.1665114473,5.2912544178
H,0,-0.5534849996,-2.2743815472,6.0784898075
H,0,-0.3967321101,-2.972634983,4.4531198934
H,0,1.0486473469,-2.6484199654,5.4316789785
H,0,2.7800252524,-1.4916292751,0.0178968853
H,0,2.5944538308,-2.68044656,1.3145221488
H,0,1.2406001891,-1.6218181031,0.8971427866

B3LYP/6-31G*
E(RB3LYP) = -337.714005847

Zero-point correction= 0.204478 (Hartree/Particle)
Thermal correction to Energy= 0.215541
Thermal correction to Enthalpy= 0.216485
Thermal correction to Gibbs Free Energy= 0.168441
Sum of electronic and ZPE= -337.509528
Sum of electronic and thermal Energies= -337.498465
Sum of electronic and thermal Enthalpies= -337.497521
Sum of electronic and thermal Free Energies= -337.545565

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.254	39.574	101.118

C,0,2.4491054693,0.812554677,1.5258310452
C,0,2.830634195,-0.6209496073,2.0283058973
C,0,2.2102894272,-0.8561560764,3.4123259205
O,0,0.7938095208,-0.7843306915,3.3229573157
H,0,2.8422128239,1.6043176593,2.1771623527
B,0,4.3877610263,-0.4766694366,2.0869639663
C,0,2.3271218921,-1.669221709,1.0162589817
H,0,1.3575462645,0.9017146073,1.5252390995
H,0,2.8112891881,0.9937695979,0.5081550221
H,0,4.9442095438,-0.1372259508,3.0939244057
H,0,2.5768588437,-0.0991451486,4.1266084197
H,0,5.0411750581,-0.6099892578,1.0917352156
H,0,2.5236315557,-1.8420083312,3.7928010817
C,0,0.1129014623,-0.8614090684,4.566466793
H,0,-0.9008385421,-0.4980554706,4.3641707821
C,0,0.0497993388,-2.2742347644,5.1473234088
H,0,0.5737296904,-0.1699618978,5.2920487709
H,0,-0.5650956002,-2.2822264358,6.0551180208
H,0,-0.3960272934,-2.963322467,4.4221902879
H,0,1.0420584878,-2.6526982747,5.4148914074
H,0,2.7659773723,-1.5021224301,0.0262658903
H,0,2.5980514072,-2.6848811227,1.3313964413
H,0,1.2364328685,-1.6318794008,0.9243424736

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.196299	E(Thermal)=	0.207684
E(QCISD(T))=	-336.615268	E(Empiric)=	-0.162240
DE(Plus)=	-0.020435	DE(2DF)=	-0.327305
E(Delta-G3)=	-0.459139	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.388089	G3 Energy=	-337.376704
G3 Enthalpy=	-337.375759	G3 Free Energy=	-337.424469

6e-22 Product
B3LYP/6-31+G**
E(RB3LYP) = -337.748280704

Zero-point correction= 0.202681 (Hartree/Particle)
Thermal correction to Energy= 0.213870
Thermal correction to Enthalpy= 0.214814
Thermal correction to Gibbs Free Energy= 0.166463
Sum of electronic and ZPE= -337.545600

Sum of electronic and thermal Energies= -337.534411
Sum of electronic and thermal Enthalpies= -337.533466
Sum of electronic and thermal Free Energies= -337.581817

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.206	39.804	101.763

O,0,1.064435338,0.5862892757,2.559343812
C,0,1.7959921181,-0.6155100613,2.3373790139
C,0,2.0455319685,-1.2848820077,3.6939292783
C,0,0.7213306346,-1.79405126,4.2979910104
C,0,0.7812814058,1.3114435601,1.3698209874
B,0,2.8383885677,-0.3061179416,4.6395972688
H,0,1.2249796174,-1.2813490791,1.6650948967
H,0,3.6928785353,0.3993916739,4.18683813
H,0,2.7539300191,-0.3809219963,1.8443638578
H,0,2.6754854394,-0.32116419,5.8257094186
C,0,3.0159800815,-2.4844192235,3.4853634512
H,0,0.8911156376,-2.2677610588,5.2709574707
H,0,0.013513453,-0.9725386988,4.44141328
H,0,0.246144099,-2.5350432607,3.6402447579
H,0,0.1986322106,0.6785291319,0.6798434823
C,0,0.0023590498,2.5648395016,1.7329619353
H,0,1.7235254129,1.5736573169,0.8604546351
H,0,3.2244932538,-2.99904703,4.4299590476
H,0,2.5590516554,-3.2209851675,2.8108053103
H,0,3.9725388024,-2.1784431375,3.0463834135
H,0,-0.2269784616,3.1426712153,0.8312115587
H,0,-0.9390791078,2.3051244381,2.226815407
H,0,0.5837762693,3.1972929993,2.4109175763

B3LYP/6-31G*
E(RB3LYP) = -337.715737811

Zero-point correction= 0.204916 (Hartree/Particle)
Thermal correction to Energy= 0.215445
Thermal correction to Enthalpy= 0.216389
Thermal correction to Gibbs Free Energy= 0.170187
Sum of electronic and ZPE= -337.510822
Sum of electronic and thermal Energies= -337.500293
Sum of electronic and thermal Enthalpies= -337.499349
Sum of electronic and thermal Free Energies= -337.545551

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.194	38.879	97.240

O,0,1.5072153892,0.5117594906,1.2993944098
C,0,2.2203318466,-0.6038768924,1.8103852447
C,0,2.1004043791,-0.7640240197,3.3502401565
C,0,0.6183599522,-0.9272806823,3.7371144028
C,0,2.0647462331,1.7539064451,1.6579534275
B,0,2.82410277,0.4235825281,4.0917570088
H,0,1.7804813366,-1.4782143736,1.3147585422
H,0,3.9684726043,0.6702592999,3.8305025004
H,0,3.2819005287,-0.5409251654,1.5188304295
H,0,2.303115614,1.0270393459,4.987101149
C,0,2.8895397845,-2.0485891938,3.7288907937
C,0,1.1984762794,2.867669714,1.0929656055
H,0,2.1105402054,1.8548094488,2.7696355058
H,0,3.103012321,1.8326684525,1.2967906312
H,0,1.6060566756,3.8468675227,1.36548949
H,0,1.1587022226,2.7970843818,0.00120541
H,0,0.1773370773,2.7930603187,1.4796128382
H,0,2.8523859754,-2.2425703369,4.80731635
H,0,2.4500826007,-2.9225058063,3.2279360321
H,0,3.9441391114,-1.9861749563,3.436469646
H,0,0.5032338789,-1.0454778297,4.8207175431
H,0,0.0325922749,-0.0550495842,3.4301411967
H,0,0.1745219392,-1.8091601076,3.2538776868

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.196723	E(Thermal)=	0.207581
E(QCISD(T))=	-336.617655	E(Empiric)=	-0.162240
DE(Plus)=	-0.020717	DE(2DF)=	-0.328330
E(Delta-G3)=	-0.459030	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.391249	G3 Energy=	-337.380391
G3 Enthalpy=	-337.379447	G3 Free Energy=	-337.426296

6e-23 Product
B3LYP/6-31+G**
E(RB3LYP) = -337.747187714

Zero-point correction= 0.202752 (Hartree/Particle)
Thermal correction to Energy= 0.213909

Thermal correction to Enthalpy= 0.214853
Thermal correction to Gibbs Free Energy= 0.166787
Sum of electronic and ZPE= -337.544435
Sum of electronic and thermal Energies= -337.533279
Sum of electronic and thermal Enthalpies= -337.532334
Sum of electronic and thermal Free Energies= -337.580401

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	134.230	39.856	101.165

C,0,2.4634368755,1.0137260204,1.6422025751
C,0,2.9858825636,-0.2210009527,2.4050218622
C,0,2.2474030909,-0.4009039539,3.7376066158
O,0,0.850277249,-0.5560004028,3.5171199713
H,0,2.6075278998,1.930587608,2.2266563061
B,0,4.5409875942,-0.254101327,2.5805845742
C,0,2.7905158409,-1.5002236228,1.5213156698
H,0,1.3928538933,0.9197364983,1.4325579909
H,0,2.9938594675,1.1397824673,0.6924400907
H,0,5.2479036069,0.1868214671,1.7216102049
H,0,2.4193727606,0.4772490434,4.3843795296
H,0,5.049268065,-0.7987322873,3.5192269854
H,0,2.638944129,-1.2832587316,4.2706586759
C,0,0.1020635506,-0.7050178632,4.715170982
C,0,-1.3665561661,-0.8690812743,4.3597030437
H,0,0.4652092223,-1.58270249,5.276180985
H,0,0.2485256175,0.1786280612,5.3591251177
H,0,3.2874244159,-1.4000288049,0.5505549913
H,0,3.1653511031,-2.4084117736,2.0093809718
H,0,1.7192276148,-1.6420031877,1.3432831456
H,0,-1.9661445534,-0.9857817384,5.2688932029
H,0,-1.7316467468,0.0064016134,3.8138556071
H,0,-1.5150590938,-1.7527123689,3.7312509011

B3LYP/6-31G*
E(RB3LYP) = -337.716190238

Zero-point correction= 0.204329 (Hartree/Particle)
Thermal correction to Energy= 0.215442
Thermal correction to Enthalpy= 0.216387
Thermal correction to Gibbs Free Energy= 0.168404
Sum of electronic and ZPE= -337.511861
Sum of electronic and thermal Energies= -337.500748

Sum of electronic and thermal Enthalpies= -337.499804
Sum of electronic and thermal Free Energies= -337.547786

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	135.192	39.570	100.987

C,0,2.4570849525,1.0135437856,1.6518522315
C,0,2.987637243,-0.2183172825,2.4118197601
C,0,2.2522355464,-0.394557556,3.7465883344
O,0,0.8604920419,-0.551712168,3.5180901769
H,0,2.614396524,1.9325941061,2.2304382068
B,0,4.5435450708,-0.2584143223,2.5722774686
C,0,2.7779140273,-1.5001094755,1.5355588978
H,0,1.3822645218,0.9223555015,1.4622763923
H,0,2.970782493,1.1354549888,0.6917416872
H,0,5.2474495996,0.1804005184,1.7079873551
H,0,2.4246358754,0.4851518474,4.3922450776
H,0,5.0587939411,-0.8095230643,3.5046696004
H,0,2.6468074274,-1.2732079427,4.2851958183
C,0,0.1086858049,-0.7045111299,4.7084585438
C,0,-1.3563840783,-0.8697857783,4.3379528608
H,0,0.4665880598,-1.5823932317,5.2740932333
H,0,0.2466221515,0.1757055274,5.3602824
H,0,3.2412724162,-1.3963480575,0.5483455388
H,0,3.1808746147,-2.4036605681,2.0114666465
H,0,1.7025895181,-1.6550709769,1.3967823094
H,0,-1.9684919434,-0.9911010463,5.2384925887
H,0,-1.7148027833,0.0073457654,3.7894205741
H,0,-1.4943650242,-1.7508674406,3.7027442975

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.196156	E(Thermal)=	0.207589
E(QCISD(T))=	-336.617306	E(Empiric)=	-0.162240
DE(Plus)=	-0.020592	DE(2DF)=	-0.327082
E(Delta-G3)=	-0.459386	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.390450	G3 Energy=	-337.379016
G3 Enthalpy=	-337.378072	G3 Free Energy=	-337.426719

6e-25 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -337.673148187

Zero-point correction= 0.198680 (Hartree/Particle)
Thermal correction to Energy= 0.210494
Thermal correction to Enthalpy= 0.211438
Thermal correction to Gibbs Free Energy= 0.159960
Sum of electronic and ZPE= -337.474468
Sum of electronic and thermal Energies= -337.462654
Sum of electronic and thermal Enthalpies= -337.461710
Sum of electronic and thermal Free Energies= -337.513188

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	132.087	39.749	108.345

C,0,-0.18549,0.05356,-0.90928
C,0,-0.45833,1.02841,-0.01545
C,0,0.04624,1.23158,1.39434
C,0,1.4249,-1.45722,0.17766
B,0,-3.05104,-1.37757,0.19078
H,0,-0.65221,0.11889,-1.88883
H,0,-2.41742,-2.35541,-0.06761
H,0,-3.09116,-0.96972,1.31314
H,0,-3.69374,-0.83935,-0.65992
C,0,-1.37036,2.14698,-0.47941
H,0,-0.79159,1.20873,2.10481
H,0,0.78099,0.50363,1.7345
H,0,0.50037,2.22854,1.48821
H,0,1.61449,-2.52035,-0.00053
C,0,2.74579,-0.69432,0.19955
H,0,0.88257,-1.3799,1.12622
H,0,-2.23516,2.26084,0.18862
H,0,-0.83986,3.11043,-0.47237
H,0,-1.75071,1.98205,-1.49231
H,0,3.38323,-1.0672,1.01
H,0,3.27546,-0.83526,-0.74803
H,0,2.5946,0.37893,0.34856
O,0,0.58672,-1.06986,-0.91219

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.190733	E(Thermal)=	0.202841
E(QCISD(T))=	-336.568750	E(Empiric)=	-0.162240
DE(Plus)=	-0.020686	DE(2DF)=	-0.325533
E(Delta-G3)=	-0.460786	E(G3-Empiric)=	-0.162240
G3(0 K)=	-337.347262	G3 Energy=	-337.335154

G3 Enthalpy= -337.334210 G3 Free Energy= -337.386355

6f-1 Starting Material
B3LYP/6-31+G**
E(RB3LYP) = -349.203508034

Zero-point correction= 0.179065 (Hartree/Particle)
Thermal correction to Energy= 0.186988
Thermal correction to Enthalpy= 0.187932
Thermal correction to Gibbs Free Energy= 0.146965
Sum of electronic and ZPE= -349.024443
Sum of electronic and thermal Energies= -349.016520
Sum of electronic and thermal Enthalpies= -349.015576
Sum of electronic and thermal Free Energies= -349.056543

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	117.337	30.429	86.222

C,0,2.2010649842,0.6748482485,1.1984190001
C,0,2.6095414104,-0.5749908413,1.9475612763
C,0,1.9898741529,-0.9781937361,3.0707605375
C,0,0.8245903409,-0.2548846027,3.6959782291
C,0,0.2001762786,0.7707537045,2.7384335788
C,0,1.2875531282,1.588293479,2.0301257052
H,0,1.168934484,0.238485858,4.6164771537
H,0,3.432084645,-1.1496046103,1.5334292616
H,0,1.6909672513,0.3967572702,0.2624325904
H,0,0.082953144,-0.9987813765,4.0111047283
H,0,-0.4042478217,0.2460853843,1.9858221221
H,0,-0.4828357203,1.426262884,3.2910583978
H,0,1.8891305939,2.1148563873,2.7840626115
H,0,0.8382352708,2.3561496747,1.3891677078
H,0,3.0987460769,1.2279027171,0.8911936886
O,0,2.3194858395,-2.0837448599,3.8139885322
C,0,3.4298184251,-2.8647937636,3.3970590982
H,0,3.5270114376,-3.667594461,4.1295611304
H,0,3.2616441952,-3.2958898936,2.40158038
H,0,4.3508608836,-2.2676844622,3.3798552704

B3LYP/6-31G*
E(RB3LYP) = -349.175157391

Zero-point correction= 0.180357 (Hartree/Particle)
Thermal correction to Energy= 0.188232
Thermal correction to Enthalpy= 0.189176
Thermal correction to Gibbs Free Energy= 0.148280
Sum of electronic and ZPE= -348.994801
Sum of electronic and thermal Energies= -348.986926
Sum of electronic and thermal Enthalpies= -348.985982
Sum of electronic and thermal Free Energies= -349.026877

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	118.117	30.137	86.072

C,0,2.2034598718,0.6728372149,1.2011723766
C,0,2.6085279436,-0.5764280197,1.9502550076
C,0,1.9910454697,-0.9795436971,3.0719083956
C,0,0.8269004489,-0.253363889,3.6979784275
C,0,0.2010406094,0.7671829258,2.7370956549
C,0,1.2883102937,1.5858834864,2.0311452354
H,0,1.1701223724,0.245009277,4.6168831349
H,0,3.4309120291,-1.1515640785,1.5350322961
H,0,1.6957610212,0.3971189407,0.2622660012
H,0,0.085435004,-0.9958926861,4.0188791061
H,0,-0.398937615,0.2381246026,1.9836003557
H,0,-0.4869339338,1.4218825804,3.2855751807
H,0,1.8882367707,2.1123877692,2.786662055
H,0,0.8397191985,2.3544248919,1.3897477774
H,0,3.1017295229,1.2272745686,0.8951104016
O,0,2.316592502,-2.0831777391,3.8161217002
C,0,3.4238613396,-2.8596413374,3.3944061918
H,0,3.5289217265,-3.6637775123,4.1257692417
H,0,3.2552333487,-3.2919393165,2.3986631974
H,0,4.3456510761,-2.2625649816,3.3697992627

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.173143	E(Thermal)=	0.181287
E(QCISD(T))=	-348.097664	E(Empiric)=	-0.155480
DE(Plus)=	-0.020611	DE(2DF)=	-0.309172
E(Delta-G3)=	-0.463128	E(G3-Empiric)=	-0.155480
G3(0 K)=	-348.872912	G3 Energy=	-348.864767
G3 Enthalpy=	-348.863823	G3 Free Energy=	-348.905200

For Anharmonic Corrections 6f-1

Zero-point vibrational energy 473525.6 (Joules/Mol)
113.17534 (Kcal/Mol)
Warning -- explicit consideration of 10 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 132.73 237.17 312.23 367.76 402.17
(Kelvin) 465.20 574.64 667.74 719.54 762.52
926.20 1136.99 1162.78 1221.16 1255.00
1344.90 1363.18 1405.19 1523.85 1555.47
1590.11 1602.64 1689.06 1707.11 1725.46
1752.74 1804.62 1842.93 1884.17 1941.89
1994.83 2004.74 2015.78 2050.05 2155.55
2168.46 2181.37 2184.00 2187.98 2206.48
2212.50 2503.12 4308.29 4347.66 4351.19
4358.56 4368.77 4381.88 4420.29 4428.22
4430.24 4437.95 4533.45 4595.45

Zero-point correction= 0.180356 (Hartree/Particle)
Thermal correction to Energy= 0.188231
Thermal correction to Enthalpy= 0.189175
Thermal correction to Gibbs Free Energy= 0.148280
Sum of electronic and zero-point Energies= -348.994801
Sum of electronic and thermal Energies= -348.986926
Sum of electronic and thermal Enthalpies= -348.985982
Sum of electronic and thermal Free Energies= -349.026877

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	118.117	30.137	86.072

ZPE(harm) = 0.47353D+03 kJ/mol ZPE(anh)= 0.46622D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.39618D-81	0.86213D-80	
QZvib	0.35966D+02	0.41113D+02	
Energy	0.49420D+03	0.48726D+03	kJ/mol
Enthalpy	0.49668D+03	0.48974D+03	kJ/mol
Entropy	0.36012D+03	0.36244D+03	J/(mol K)
Sp.Heat(V)	0.12609D+03	0.12884D+03	J/(mol K)
Sp.Heat(P)	0.13441D+03	0.13715D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.39618D-81	0.86213D-80	
QZvib	0.35966D+02	0.41113D+02	
Energy	0.49420D+03	0.48726D+03	kJ/mol
Enthalpy	0.49668D+03	0.48974D+03	kJ/mol
Entropy	0.36012D+03	0.36244D+03	J/(mol K)
Sp.Heat(V)	0.12609D+03	0.12884D+03	J/(mol K)
Sp.Heat(P)	0.13441D+03	0.13715D+03	J/(mol K)

6f-2 Starting Material

B3LYP/6-31+G**

E(RB3LYP) = -349.196512767

Zero-point correction= 0.178514 (Hartree/Particle)
Thermal correction to Energy= 0.186686
Thermal correction to Enthalpy= 0.187630
Thermal correction to Gibbs Free Energy= 0.145657
Sum of electronic and ZPE= -349.017999
Sum of electronic and thermal Energies= -349.009827
Sum of electronic and thermal Enthalpies= -349.008882
Sum of electronic and thermal Free Energies= -349.050856

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	117.147	30.665	88.340

C,0,2.1357568328,0.4456126334,1.2146118531
C,0,2.6006685457,-0.5572615322,2.2428885806
C,0,2.0683740743,-0.6560743663,3.4693062133
C,0,0.9094007058,0.1854115862,3.9501662259
C,0,0.2280305153,0.9367500782,2.7927171528
C,0,1.260846231,1.5448548049,1.8368644842
H,0,1.2795809049,0.8945295126,4.7063234267
H,0,3.4330350094,-1.2112646978,1.9938418854
H,0,1.5762826509,-0.0685608248,0.4172306014
H,0,0.1669501873,-0.4385648701,4.4621910866
H,0,-0.4093228175,0.2375505704,2.234327974
H,0,-0.4334948628,1.7116412546,3.1974031246
H,0,1.8988033678,2.2453056693,2.3932845903
H,0,0.7626496034,2.1243088581,1.0505512364
H,0,3.0069400519,0.8947823378,0.7193065981

O,0,2.6856139722,-1.4934193147,4.3836547922
C,0,1.8558781861,-2.3399346182,5.1748742655
H,0,2.5327960205,-3.0154925877,5.7016711614
H,0,1.2735943077,-1.7780535181,5.9154858637
H,0,1.1752015136,-2.9310119755,4.5472948836

E(RB3LYP) = -349.168220918

Zero-point correction= 0.179814 (Hartree/Particle)
Thermal correction to Energy= 0.187937
Thermal correction to Enthalpy= 0.188882
Thermal correction to Gibbs Free Energy= 0.146969
Sum of electronic and ZPE= -348.988407
Sum of electronic and thermal Energies= -348.980284
Sum of electronic and thermal Enthalpies= -348.979339
Sum of electronic and thermal Free Energies= -349.021252

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	117.933	30.378	88.213

C,0,2.1417077279,0.459093565,1.2117071883
C,0,2.6004851956,-0.5589256923,2.2260242888
C,0,2.0667180712,-0.6771753165,3.4485721768
C,0,0.9041067162,0.1559516839,3.936387971
C,0,0.228332168,0.9232199544,2.787019057
C,0,1.265330895,1.5484216161,1.8479376909
H,0,1.2656309397,0.8544321428,4.7072267559
H,0,3.4324528136,-1.2103465652,1.9679395877
H,0,1.5845165054,-0.0404073504,0.4023065882
H,0,0.1581117624,-0.4761342981,4.4350370591
H,0,-0.4029205349,0.2303102947,2.2135367353
H,0,-0.4393137332,1.6894481242,3.1992894465
H,0,1.9009992708,2.2384151478,2.4201523562
H,0,0.7711701638,2.1424450701,1.0693932521
H,0,3.0147400161,0.916538012,0.7256036357
O,0,2.6823099801,-1.5307024639,4.3441433345
C,0,1.8563430971,-2.316069693,5.1916215847
H,0,2.5268701136,-3.0090332686,5.7056911373
H,0,1.3322535784,-1.7136024331,5.9453386139
H,0,1.1177402533,-2.8947695299,4.61906754

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203852	E(Thermal)=	0.214351

E(QCISD(T))=	-374.599491	E(Empiric)=	-0.175760
DE(Plus)=	-0.020832	DE(2DF)=	-0.351754
E(Delta-G3)=	-0.511603	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.455589	G3 Energy=	-375.445090
G3 Enthalpy=	-375.444146	G3 Free Energy=	-375.490369

For Anharmonic Corrections of 6f-2

Zero-point correction= 0.179813 (Hartree/Particle)
Thermal correction to Energy= 0.187937
Thermal correction to Enthalpy= 0.188881
Thermal correction to Gibbs Free Energy= 0.146968
Sum of electronic and zero-point Energies= -348.988408
Sum of electronic and thermal Energies= -348.980284
Sum of electronic and thermal Enthalpies= -348.979340
Sum of electronic and thermal Free Energies= -349.021253

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.932	30.378	88.214

omecyclo_temp9_anahrmonic 4f-12
Zero-point correction= 0.211992 (Hartree/Particle)
Thermal correction to Energy= 0.221046
Thermal correction to Enthalpy= 0.221990
Thermal correction to Gibbs Free Energy= 0.178718
Sum of electronic and zero-point Energies= -375.569357
Sum of electronic and thermal Energies= -375.560302
Sum of electronic and thermal Enthalpies= -375.559358
Sum of electronic and thermal Free Energies= -375.602631

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.708	36.203	91.074

omecyclo_tempcom7_anharmonic 4f-6
Zero-point correction= 0.212308 (Hartree/Particle)
Thermal correction to Energy= 0.222456
Thermal correction to Enthalpy= 0.223400
Thermal correction to Gibbs Free Energy= 0.177812

Sum of electronic and zero-point Energies= -375.589357
Sum of electronic and thermal Energies= -375.579208
Sum of electronic and thermal Enthalpies= -375.578264
Sum of electronic and thermal Free Energies= -375.623853

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.593	38.971	95.950

6f-3 Complex
B3LYP/6-31+G**
E(RB3LYP) = -375.835347406

Zero-point correction= 0.210963 (Hartree/Particle)
Thermal correction to Energy= 0.221178
Thermal correction to Enthalpy= 0.222122
Thermal correction to Gibbs Free Energy= 0.176714
Sum of electronic and ZPE= -375.624384
Sum of electronic and thermal Energies= -375.614169
Sum of electronic and thermal Enthalpies= -375.613225
Sum of electronic and thermal Free Energies= -375.658633

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	138.791	39.433	95.569

C,0,2.0074129331,0.5790471594,1.167571371
C,0,2.2724220444,-0.7710879529,1.8358990912
C,0,1.8361483397,-1.0088264171,3.1229240113
C,0,0.7997952295,-0.1657845765,3.8174179189
C,0,0.2829427553,1.0048596032,2.9662886222
C,0,1.4195621564,1.6154183468,2.1377475827
B,0,0.861090367,-2.0266001742,1.2462131275
H,0,1.2779495649,0.2047564432,4.7345070672
H,0,3.1468418327,-1.3102517267,1.4876816283
H,0,1.334170762,0.4436757545,0.3142057086
H,0,-0.0171273653,-0.8203271915,4.1418257028
H,0,-0.5067398711,0.6515352748,2.2951722527
H,0,-0.1661135595,1.7556519265,3.625922767
H,0,2.2074937366,1.977689238,2.8138810496
H,0,1.0602118501,2.4858182146,1.5772093682

H,0,2.9551454397,0.9498816809,0.7583394343
H,0,-0.1830229942,-1.4628996395,1.4319027033
H,0,1.2536990476,-2.0163468673,0.1073946332
H,0,1.0068542126,-3.0699042326,1.8265092581
O,0,2.2881170163,-1.9712844275,3.9382435374
C,0,3.3598628981,-2.8238990611,3.5122475788
H,0,3.5515905079,-3.4883539713,4.3544341075
H,0,3.0577650045,-3.4037104267,2.6365157391
H,0,4.255937092,-2.2342079766,3.2905167392

B3LYP/6-31G*
E(RB3LYP) = -375.805368068

Zero-point correction= 0.212542 (Hartree/Particle)
Thermal correction to Energy= 0.222668
Thermal correction to Enthalpy= 0.223612
Thermal correction to Gibbs Free Energy= 0.178383
Sum of electronic and ZPE= -375.592826
Sum of electronic and thermal Energies= -375.582700
Sum of electronic and thermal Enthalpies= -375.581756
Sum of electronic and thermal Free Energies= -375.626985

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.726	39.071	95.192

C,0,2.0132441009,0.5802897937,1.168854655
C,0,2.2777773166,-0.7694114355,1.8372735573
C,0,1.8400631728,-1.0106843766,3.1222762927
C,0,0.8027134933,-0.1662476384,3.8165693983
C,0,0.2809889167,0.9984086853,2.9613726176
C,0,1.4168830871,1.6139237055,2.1364700297
B,0,0.8602513105,-2.0199699656,1.2553834031
H,0,1.2823789806,0.2111073069,4.7307729648
H,0,3.1518226865,-1.3096420292,1.4882270583
H,0,1.3462188058,0.4436652147,0.3105824757
H,0,-0.0118606394,-0.8202753896,4.1485865638
H,0,-0.5028740809,0.636324782,2.2878468857
H,0,-0.1768718152,1.7479681875,3.6171827285
H,0,2.2009582857,1.9796357535,2.8156476332
H,0,1.0558110346,2.4834039327,1.5747508544
H,0,2.9624572221,0.9556163156,0.7654719679
H,0,-0.1855528126,-1.458086882,1.4438448995
H,0,1.2516462168,-2.008045386,0.1154397578

H,0,1.0061478707,-3.0651419441,1.8346574032
O,0,2.2876824167,-1.9719216604,3.9388583449
C,0,3.3536740039,-2.824310275,3.5082363087
H,0,3.5519966094,-3.4885865719,4.3500155656
H,0,3.0458524619,-3.4050480861,2.634667561
H,0,4.2506003556,-2.2381230369,3.2775820733

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.204040	E(Thermal)=	0.214519
E(QCISD(T))=	-374.602484	E(Empiric)=	-0.175760
DE(Plus)=	-0.021262	DE(2DF)=	-0.352337
E(Delta-G3)=	-0.511747	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.459550	G3 Energy=	-375.449072
G3 Enthalpy=	-375.448128	G3 Free Energy=	-375.494014

For Anharmonic Corrections of 6f-3

Zero-point vibrational energy 558028.4 (Joules/Mol)
133.37200 (Kcal/Mol) Warning -- explicit consideration of 14 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 177.35 182.53 242.89 294.67 298.37
(Kelvin) 348.60 361.99 401.20 431.06 499.07
593.13 692.56 729.26 762.45 908.24
1098.40 1135.99 1185.06 1212.57 1259.10
1325.77 1348.07 1377.64 1407.91 1499.15
1553.77 1577.73 1610.90 1625.77 1695.71
1703.96 1715.97 1727.92 1735.19 1756.78
1835.78 1853.55 1892.64 1937.83 1991.10
2007.77 2021.16 2054.96 2136.77 2147.79
2184.18 2186.69 2191.30 2208.36 2210.19
2347.96 3620.41 3728.82 3756.49 4354.55
4376.06 4388.07 4399.63 4409.30 4433.56
4449.24 4452.08 4479.72 4517.66 4573.37
4606.94

Zero-point correction=	0.212542 (Hartree/Particle)
Thermal correction to Energy=	0.222668
Thermal correction to Enthalpy=	0.223612
Thermal correction to Gibbs Free Energy=	0.178383
Sum of electronic and zero-point Energies=	-375.592826
Sum of electronic and thermal Energies=	-375.582700
Sum of electronic and thermal Enthalpies=	-375.581756
Sum of electronic and thermal Free Energies=	-375.626985

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.726	39.071	95.192

ZPE(harm) = 0.55803D+03 kJ/mol ZPE(anh)= 0.54865D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.33494D-95	0.43332D-93	
QZvib	0.19373D+03	0.56951D+03	
Energy	0.58461D+03	0.57668D+03	kJ/mol
Enthalpy	0.58709D+03	0.57916D+03	kJ/mol
Entropy	0.39828D+03	0.41211D+03	J/(mol K)
Sp.Heat(V)	0.16347D+03	0.16840D+03	J/(mol K)
Sp.Heat(P)	0.17179D+03	0.17672D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.33494D-95	0.43332D-93	
QZvib	0.19373D+03	0.56951D+03	
Energy	0.58461D+03	0.57668D+03	kJ/mol
Enthalpy	0.58709D+03	0.57916D+03	kJ/mol
Entropy	0.39828D+03	0.41211D+03	J/(mol K)
Sp.Heat(V)	0.16347D+03	0.16840D+03	J/(mol K)
Sp.Heat(P)	0.17179D+03	0.17672D+03	J/(mol K)

6f-4 Complex

B3LYP/6-31+G**

E(RB3LYP) = -375.835347378

Zero-point correction= 0.210963 (Hartree/Particle)
Thermal correction to Energy= 0.221178
Thermal correction to Enthalpy= 0.222122
Thermal correction to Gibbs Free Energy= 0.176715
Sum of electronic and ZPE= -375.624384
Sum of electronic and thermal Energies= -375.614169
Sum of electronic and thermal Enthalpies= -375.613225
Sum of electronic and thermal Free Energies= -375.658632

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	138.791	39.432	95.567

C,0,2.1337580278,0.6001607228,1.1661873667
C,0,2.3602392669,-0.7603327272,1.8276595245
C,0,1.8390613612,-1.0224076494,3.0778665223
C,0,0.7533588836,-0.1961564905,3.7147551919
C,0,0.2889918068,0.986974342,2.8507329412
C,0,1.4758117782,1.6168382432,2.1118862216
B,0,0.9992362043,-2.0113299829,1.1220922162
H,0,1.1661557487,0.1603192734,4.6684360496
H,0,3.2592758809,-1.2894686369,1.5304829465
H,0,1.5206701019,0.4768618413,0.2668915889
H,0,-0.0800712191,-0.8598129488,3.9716311199
H,0,-0.451410785,0.642050464,2.1215793096
H,0,-0.2078766991,1.7241578519,3.4911553304
H,0,2.2140885177,1.9705914773,2.8460800786
H,0,1.1505327718,2.4953736956,1.5432899767
H,0,3.1050081831,0.9821801598,0.8286662382
H,0,-0.0581683799,-1.4554590394,1.2459156555
H,0,1.4681371936,-1.9796600539,0.0128994004
H,0,1.1108912864,-3.063976328,1.6930209703
O,0,2.2400462231,-1.9969645404,3.9053698314
C,0,3.342826493,-2.8374244081,3.5385035733
H,0,3.4806191618,-3.5157114669,4.3802149981
H,0,3.103934892,-3.4030741967,2.6344483395
H,0,4.2486523004,-2.2401296025,3.3882846083

B3LYP/6-31G*
E(RB3LYP) = -375.805367885

Zero-point correction= 0.212545 (Hartree/Particle)
Thermal correction to Energy= 0.222669
Thermal correction to Enthalpy= 0.223613
Thermal correction to Gibbs Free Energy= 0.178390
Sum of electronic and ZPE= -375.592823
Sum of electronic and thermal Energies= -375.582699
Sum of electronic and thermal Enthalpies= -375.581755
Sum of electronic and thermal Free Energies= -375.626978

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.727	39.068	95.180

C,0,2.1392310732,0.6010964549,1.1678110501
C,0,2.3649573717,-0.7591928497,1.8291073678

C,0,1.8429983362,-1.0242881147,3.0774937176
C,0,0.7560768877,-0.1968314225,3.7140056626
C,0,0.2875022853,0.9806715122,2.8456865794
C,0,1.4735496174,1.6151147175,2.1106210765
B,0,0.9976967323,-2.0044948428,1.1308094845
H,0,1.1699989367,0.1660813967,4.6653998479
H,0,3.2637810532,-1.2893412928,1.5312517338
H,0,1.5323558657,0.4769615951,0.2642112525
H,0,-0.0756164182,-0.860307947,3.9778578631
H,0,-0.4470121442,0.6274489545,2.1143140119
H,0,-0.217613644,1.7167058381,3.4818223808
H,0,2.2079779671,1.9717228371,2.8476818378
H,0,1.1469978903,2.4930208695,1.5409386549
H,0,3.1115560457,0.9872543324,0.8360594754
H,0,-0.0613974027,-1.4501526258,1.2574941012
H,0,1.4656044156,-1.9713537584,0.0204866645
H,0,1.1086862868,-3.0592284161,1.7005542852
O,0,2.2398704519,-1.9973333204,3.906126709
C,0,3.3373232818,-2.8373126055,3.5344852725
H,0,3.4823693656,-3.5147992135,4.3766086978
H,0,3.0924875576,-3.4046474924,2.6326606601
H,0,4.2443871873,-2.2431946065,3.3745616129

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.204043	E(Thermal)=	0.214520
E(QCISD(T))=	-374.602483	E(Empiric)=	-0.175760
DE(Plus)=	-0.021262	DE(2DF)=	-0.352338
E(Delta-G3)=	-0.511747	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.459547	G3 Energy=	-375.449071
G3 Enthalpy=	-375.448126	G3 Free Energy=	-375.494007

For Anharmonic Corrections of 6f-4

Zero-point vibrational energy 558035.9 (Joules/Mol)
133.37377 (Kcal/Mol) Warning -- explicit consideration of 14 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 178.03 182.87 242.78 294.52 298.07
(Kelvin) 348.40 362.02 401.73 431.41 499.27
593.25 692.62 729.27 762.58 908.18
1098.65 1136.20 1185.17 1212.59 1259.14
1325.87 1348.13 1377.94 1407.97 1499.34
1553.81 1577.73 1610.89 1625.92 1695.73
1703.92 1715.97 1728.10 1735.21 1756.82

1835.92 1853.55 1892.64 1937.81 1991.08
2007.75 2021.16 2054.96 2136.72 2147.83
2184.17 2186.72 2191.26 2208.34 2210.18
2347.76 3620.00 3728.36 3755.84 4354.48
4376.37 4388.09 4399.59 4409.32 4433.61
4449.20 4452.17 4479.73 4517.66 4573.32
4606.73

Zero-point correction= 0.212545 (Hartree/Particle)
Thermal correction to Energy= 0.222669
Thermal correction to Enthalpy= 0.223613
Thermal correction to Gibbs Free Energy= 0.178390
Sum of electronic and zero-point Energies= -375.592823
Sum of electronic and thermal Energies= -375.582699
Sum of electronic and thermal Enthalpies= -375.581755
Sum of electronic and thermal Free Energies= -375.626978

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.727	39.068	95.179

ZPE(harm) = 0.55804D+03 kJ/mol ZPE(anh)= 0.54847D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.33257D-95	0.54747D-93	
QZvib	0.19294D+03	0.67107D+03	
Energy	0.58462D+03	0.57665D+03	kJ/mol
Enthalpy	0.58710D+03	0.57912D+03	kJ/mol
Entropy	0.39823D+03	0.41393D+03	J/(mol K)
Sp.Heat(V)	0.16346D+03	0.16861D+03	J/(mol K)
Sp.Heat(P)	0.17177D+03	0.17692D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.33257D-95	0.54747D-93	
QZvib	0.19294D+03	0.67107D+03	
Energy	0.58462D+03	0.57665D+03	kJ/mol
Enthalpy	0.58710D+03	0.57912D+03	kJ/mol
Entropy	0.39823D+03	0.41393D+03	J/(mol K)
Sp.Heat(V)	0.16346D+03	0.16861D+03	J/(mol K)
Sp.Heat(P)	0.17177D+03	0.17692D+03	J/(mol K)

6f-5 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.831124445

Zero-point correction= 0.210825 (Hartree/Particle)
Thermal correction to Energy= 0.221040
Thermal correction to Enthalpy= 0.221984
Thermal correction to Gibbs Free Energy= 0.176318
Sum of electronic and ZPE= -375.620300
Sum of electronic and thermal Energies= -375.610084
Sum of electronic and thermal Enthalpies= -375.609140
Sum of electronic and thermal Free Energies= -375.654806

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.705	39.318	96.112

C,0,2.1418207122,0.5944111187,1.2610195266
C,0,2.4894243477,-0.6201968496,2.1164779881
C,0,1.9883476086,-0.78134457,3.3947521421
C,0,0.8483833685,0.0501160128,3.9362406088
C,0,0.1918815075,0.924095086,2.8554774478
C,0,1.259309796,1.6166534726,1.9998349704
B,0,1.2790858976,-2.0933764224,1.870243665
H,0,1.2823557434,0.6900180725,4.7197916856
H,0,3.4486314071,-1.0899735701,1.9251914159
H,0,1.6519111647,0.265755297,0.339054401
H,0,0.1028265241,-0.5843335218,4.4236534545
H,0,-0.4503466633,0.3023554896,2.2227433716
H,0,-0.4538979326,1.6634995642,3.3424384646
H,0,1.8871150449,2.2391601585,2.6531735476
H,0,0.7911889297,2.294854618,1.2777858087
H,0,3.0808642635,1.0743903245,0.9580453985
H,0,0.5723404577,-1.6426586847,1.011059007
H,0,2.0764105358,-2.9467927793,1.5919108167
H,0,0.6326967643,-2.4112184158,2.8450837727
O,0,2.7097857027,-1.5454868187,4.2468825563
C,0,2.0578234114,-2.1619749006,5.3647731494
H,0,2.8210884741,-2.7793971838,5.8386222745
H,0,1.6976362514,-1.4171131271,6.0816005697
H,0,1.2311866828,-2.7931533705,5.0230789566

B3LYP/6-31G*
E(RB3LYP) = -375.801235930

Zero-point correction= 0.212346 (Hartree/Particle)
Thermal correction to Energy= 0.222495
Thermal correction to Enthalpy= 0.223440
Thermal correction to Gibbs Free Energy= 0.177872
Sum of electronic and ZPE= -375.588890
Sum of electronic and thermal Energies= -375.578740
Sum of electronic and thermal Enthalpies= -375.577796
Sum of electronic and thermal Free Energies= -375.623364

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.618	38.969	95.905

C,0,2.1426163594,0.5941060879,1.2616706669
C,0,2.4909935063,-0.6193467858,2.1179313734
C,0,1.9918668825,-0.7815206348,3.396600666
C,0,0.8516420319,0.0507533204,3.9375024631
C,0,0.1934006086,0.9208695409,2.8554968584
C,0,1.2591603255,1.6152333934,2.0001522046
B,0,1.2778184911,-2.0912491014,1.8743366484
H,0,1.2846075215,0.6921770483,4.7211470812
H,0,3.4506649215,-1.0885004266,1.9259678843
H,0,1.6520198765,0.2635529593,0.340421222
H,0,0.1068825118,-0.5834116192,4.4277665434
H,0,-0.4447679954,0.29439372,2.2227594233
H,0,-0.4569505666,1.6584522446,3.3402119018
H,0,1.8863334388,2.2387272102,2.6537063889
H,0,0.7899964845,2.2935073206,1.2781065714
H,0,3.0804397208,1.0761464921,0.9560713514
H,0,0.5688668806,-1.6393906486,1.0159778795
H,0,2.0764222778,-2.9430360726,1.5925048799
H,0,0.6304418752,-2.4126560823,2.8495005993
O,0,2.711950339,-1.5466298297,4.2449942355
C,0,2.0562682891,-2.159731819,5.358333815
H,0,2.815657253,-2.7806437309,5.8355991628
H,0,1.6943661709,-1.4155150205,6.0762439966
H,0,1.2271727957,-2.7879985663,5.0159311828

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203852	E(Thermal)=	0.214351
E(QCISD(T))=	-374.599491	E(Empiric)=	-0.175760
DE(Plus)=	-0.020832	DE(2DF)=	-0.351754
E(Delta-G3)=	-0.511603	E(G3-Empiric)=	-0.175760

G3(0 K)=	-375.455589	G3 Energy=	-375.445090
G3 Enthalpy=	-375.444146	G3 Free Energy=	-375.490369

For Anharmonic Corrections of 6f-5

Zero-point correction= 0.212346 (Hartree/Particle)
Thermal correction to Energy= 0.222496
Thermal correction to Enthalpy= 0.223440
Thermal correction to Gibbs Free Energy= 0.177872
Sum of electronic and zero-point Energies= -375.588890
Sum of electronic and thermal Energies= -375.578740
Sum of electronic and thermal Enthalpies= -375.577796
Sum of electronic and thermal Free Energies= -375.623364

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.618	38.969	95.906

6f-6 Complex
B3LYP/6-31+G**
E(RB3LYP) = -375.831590508

Zero-point correction= 0.210798 (Hartree/Particle)
Thermal correction to Energy= 0.221002
Thermal correction to Enthalpy= 0.221946
Thermal correction to Gibbs Free Energy= 0.176290
Sum of electronic and ZPE= -375.620792
Sum of electronic and thermal Energies= -375.610589
Sum of electronic and thermal Enthalpies= -375.609645
Sum of electronic and thermal Free Energies= -375.655301

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	138.681	39.303	96.091

C,0,2.2008534824,0.6291679052,1.2651213539
C,0,2.6060262586,-0.5292961039,2.162183344
C,0,1.8378152152,-0.9139380861,3.2456062501
C,0,0.7270742176,-0.0416663751,3.8000226042
C,0,0.1458924979,0.8846805225,2.7126154597
C,0,1.250666048,1.6224012999,1.9484988143

B,0,3.7409927163,0.0445679085,3.5820093352
H,0,1.1010492163,0.5486496665,4.6432211759
H,0,3.1827699785,-1.3207317363,1.6931090695
H,0,1.7084849165,0.2039395554,0.3771427755
H,0,-0.0626218884,-0.6909659074,4.191291675
H,0,-0.4465683797,0.283052999,2.0097960252
H,0,-0.5451736095,1.5946697571,3.1807638046
H,0,1.8159873718,2.2535847896,2.6433104885
H,0,0.8111940876,2.2879465754,1.1965907187
H,0,3.0981879557,1.1443755757,0.9067778092
H,0,4.7219971403,-0.5744264922,3.2673874345
H,0,3.7181166285,1.2362375301,3.4263770808
H,0,3.3864662309,-0.2560714099,4.6995122127
O,0,1.9555251445,-2.1966161472,3.6588665569
C,0,1.7143517373,-2.5234346296,5.0341735389
H,0,1.9252099549,-3.5895921278,5.1185525768
H,0,2.3918251719,-1.9559470746,5.679680436
H,0,0.6747519067,-2.3363899948,5.3210134601

B3LYP/6-31G*
E(RB3LYP) = -375.801664793

Zero-point correction= 0.212310 (Hartree/Particle)
Thermal correction to Energy= 0.222458
Thermal correction to Enthalpy= 0.223402
Thermal correction to Gibbs Free Energy= 0.177814
Sum of electronic and ZPE= -375.589355
Sum of electronic and thermal Energies= -375.579207
Sum of electronic and thermal Enthalpies= -375.578263
Sum of electronic and thermal Free Energies= -375.623851

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.594	38.971	95.949

C,0,2.2003899373,0.6266931654,1.2651901589
C,0,2.6035294029,-0.5326274991,2.1612129195
C,0,1.8352851385,-0.918883507,3.2438009616
C,0,0.7236159742,-0.0460261526,3.7973812712
C,0,0.1469196173,0.8850493941,2.7124209404
C,0,1.254800489,1.6211426222,1.9522130935
B,0,3.7369487149,0.0454344773,3.5824621273
H,0,1.0951972526,0.539487225,4.6452854929
H,0,3.1805956182,-1.3237373978,1.6912432855

H,0,1.7056551661,0.2056617039,0.3759360429
H,0,-0.069383551,-0.6958405901,4.1835783068
H,0,-0.4463571398,0.2869241765,2.0067792162
H,0,-0.5437851465,1.5956972698,3.18117605
H,0,1.8237490856,2.2456089329,2.6504425739
H,0,0.8185251188,2.2928404548,1.2032614136
H,0,3.0990177708,1.1405344658,0.9069843394
H,0,4.7191583575,-0.5705543691,3.2642978721
H,0,3.7113388754,1.2377719033,3.425646838
H,0,3.3860799298,-0.2536113997,4.7031532975
O,0,1.9576873391,-2.1978724317,3.6584062951
C,0,1.7183769488,-2.5178131831,5.031888555
H,0,1.9261526763,-3.584911433,5.121599869
H,0,2.3975303642,-1.9496363571,5.6757105709
H,0,0.6798460598,-2.3271334707,5.323552509

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203817	E(Thermal)=	0.214315
E(QCISD(T))=	-374.599661	E(Empiric)=	-0.175760
DE(Plus)=	-0.021040	DE(2DF)=	-0.351294
E(Delta-G3)=	-0.511465	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.455404	G3 Energy=	-375.444906
G3 Enthalpy=	-375.443962	G3 Free Energy=	-375.490206

For Anharmonic Corrections of 6f-6

Zero-point correction=	0.212308 (Hartree/Particle)
Thermal correction to Energy=	0.222456
Thermal correction to Enthalpy=	0.223400
Thermal correction to Gibbs Free Energy=	0.177812
Sum of electronic and zero-point Energies=	-375.589357
Sum of electronic and thermal Energies=	-375.579208
Sum of electronic and thermal Enthalpies=	-375.578264
Sum of electronic and thermal Free Energies=	-375.623853

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.593	38.971	95.950

6f-7 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.825204948

Zero-point correction= 0.210761 (Hartree/Particle)
Thermal correction to Energy= 0.219974
Thermal correction to Enthalpy= 0.220918
Thermal correction to Gibbs Free Energy= 0.177208
Sum of electronic and ZPE= -375.614443
Sum of electronic and thermal Energies= -375.605231
Sum of electronic and thermal Enthalpies= -375.604287
Sum of electronic and thermal Free Energies= -375.647997

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.036	36.474	91.995

C,0,1.4302177321,1.6529127598,2.189920742
C,0,2.1827588569,0.7394717386,1.2054038452
C,0,2.3255402835,-0.7222091037,1.6755857675
C,0,1.697660534,-1.1651586397,2.9039768996
C,0,0.7522378519,-0.2517174332,3.6719113906
C,0,0.2440904359,0.9316737202,2.8411548135
B,0,1.1427624171,-1.8122088442,1.1991095277
O,0,2.2753086387,-2.0497802981,3.7793168972
C,0,3.3804833545,-2.8582305994,3.3625515335
H,0,1.3481753792,0.1256507658,4.5134711126
H,0,3.313806248,-1.1359041146,1.4973004168
H,0,1.669380151,0.7507198982,0.2375297956
H,0,-0.0641808804,-0.8388696752,4.1029473045
H,0,-0.4593345118,0.5868255408,2.0745910448
H,0,-0.3084648243,1.6126334882,3.4985265688
H,0,2.1136999248,1.985282094,2.9845163881
H,0,1.0942166932,2.5572458048,1.6694983058
H,0,3.1832095659,1.1520005317,1.0278617016
H,0,0.2341908139,-1.279085977,0.6276855529
H,0,1.5940862418,-2.8545631761,0.8173210141
H,0,0.6122608227,-2.1095621486,2.3114820401
H,0,3.5882703645,-3.5144080662,4.2085221465
H,0,3.1240352929,-3.458444738,2.4855230503
H,0,4.2642616139,-2.2452355278,3.1544041404

B3LYP/6-31G*
E(RB3LYP) = -375.793761529

Zero-point correction= 0.212205 (Hartree/Particle)
Thermal correction to Energy= 0.221354
Thermal correction to Enthalpy= 0.222298
Thermal correction to Gibbs Free Energy= 0.178663
Sum of electronic and ZPE= -375.581557
Sum of electronic and thermal Energies= -375.572407
Sum of electronic and thermal Enthalpies= -375.571463
Sum of electronic and thermal Free Energies= -375.615099

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.902	36.085	91.839

C,0,1.4285788877,1.6509518362,2.1908699635
C,0,2.1841711714,0.7400022506,1.2069068018
C,0,2.3241704806,-0.724821947,1.669216571
C,0,1.6937478472,-1.1719018916,2.9020536632
C,0,0.7543587667,-0.2515132641,3.6723309445
C,0,0.2428809099,0.9275283608,2.8390786333
B,0,1.1532895881,-1.8075643221,1.1884351806
O,0,2.2749515315,-2.0464852208,3.7831581428
C,0,3.3720406787,-2.8568817056,3.3620992947
H,0,1.357524904,0.1295427976,4.5075873574
H,0,3.3187319807,-1.130387463,1.5032035045
H,0,1.673533162,0.7561600189,0.2372974604
H,0,-0.0598654015,-0.8341952487,4.1149922531
H,0,-0.4567998135,0.5774559012,2.0708832675
H,0,-0.3150718035,1.6078316975,3.4935039556
H,0,2.1095828783,1.9836171958,2.9879345107
H,0,1.0922621826,2.556227049,1.6712392978
H,0,3.1846373689,1.1553981871,1.0327214459
H,0,0.2286246076,-1.2843312182,0.6318180371
H,0,1.5931652518,-2.8592118053,0.8163922887
H,0,0.6293009381,-2.0960212607,2.3187367736
H,0,3.5868588206,-3.5112609484,4.2088820201
H,0,3.1098331157,-3.4610982829,2.488770722
H,0,4.2581649464,-2.2500027161,3.1419999101

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203717	E(Thermal)=	0.213201
E(QCISD(T))=	-374.593285	E(Empiric)=	-0.175760
DE(Plus)=	-0.021178	DE(2DF)=	-0.352946
E(Delta-G3)=	-0.511041	E(G3-Empiric)=	-0.175760

G3(0 K)= -375.450493 G3 Energy= -375.441008
G3 Enthalpy= -375.440064 G3 Free Energy= -375.484300

For Anharmonic Correction Of 6f-10

Zero-point vibrational energy 557144.7 (Joules/Mol) 133.16077 (Kcal/Mol)
Warning -- explicit consideration of 13 degrees of freedom as vibrations may cause significant error
Vibrational temperatures: 127.61 161.93 251.58 287.51 381.31 (Kelvin) 441.01 493.91 522.85 629.99 671.23
692.92 814.57 851.92 980.06 1068.31
1175.24 1202.76 1231.83 1274.48 1352.52
1361.28 1403.09 1461.37 1515.21 1555.62
1586.07 1630.62 1652.96 1665.72 1700.08
1718.06 1729.17 1738.71 1756.17 1807.38
1862.57 1889.45 1918.15 1984.16 2001.58
2013.47 2022.73 2092.65 2160.19 2179.99
2189.51 2190.64 2191.96 2206.94 2215.00
3190.79 3683.72 3812.70 4350.48 4383.62
4386.09 4390.01 4398.42 4422.91 4442.73
4456.81 4470.25 4500.68 4552.79 4562.01

Zero-point correction= 0.212205 (Hartree/Particle)
Thermal correction to Energy= 0.221355
Thermal correction to Enthalpy= 0.222299
Thermal correction to Gibbs Free Energy= 0.178663
Sum of electronic and zero-point Energies= -375.581556
Sum of electronic and thermal Energies= -375.572407
Sum of electronic and thermal Enthalpies= -375.571463
Sum of electronic and thermal Free Energies= -375.615099

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.902	36.086	91.840

ZPE(harm) = 0.55714D+03 kJ/mol ZPE(anh)= 0.54838D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.25992D-95	0.12698D-93	
QZvib	0.10526D+03	0.14995D+03	
Energy	0.58117D+03	0.57309D+03	kJ/mol
Enthalpy	0.58365D+03	0.57557D+03	kJ/mol
Entropy	0.39257D+03	0.39784D+03	J/(mol K)

Sp.Heat(V)	0.15098D+03	0.15522D+03	J/(mol K)
Sp.Heat(P)	0.15930D+03	0.16353D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.25992D-95	0.12698D-93	
QZvib	0.10526D+03	0.14995D+03	
Energy	0.58117D+03	0.57309D+03	kJ/mol
Enthalpy	0.58365D+03	0.57557D+03	kJ/mol
Entropy	0.39257D+03	0.39784D+03	J/(mol K)
Sp.Heat(V)	0.15098D+03	0.15522D+03	J/(mol K)
Sp.Heat(P)	0.15930D+03	0.16353D+03	J/(mol K)

6f-8 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.813825999

Zero-point correction= 0.210566 (Hartree/Particle)
Thermal correction to Energy= 0.219695
Thermal correction to Enthalpy= 0.220639
Thermal correction to Gibbs Free Energy= 0.177252
Sum of electronic and ZPE= -375.603260
Sum of electronic and thermal Energies= -375.594131
Sum of electronic and thermal Enthalpies= -375.593187
Sum of electronic and thermal Free Energies= -375.636574

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.861	36.529	91.316

C,0,2.0928403808,0.7190441747,1.2084889725
C,0,2.3209875095,-0.6951032531,1.7552742167
C,0,1.6359612458,-1.1723574166,2.9263746581
C,0,0.7483129275,-0.2333247893,3.7365136778
C,0,0.298660736,1.0140945527,2.9643347272
C,0,1.4921037011,1.6670573131,2.2588342754
B,0,0.9424949686,-1.890913932,1.5589247963
H,0,1.3375348033,0.0776160324,4.6097826885
H,0,3.2938034065,-1.1270516494,1.538709573
H,0,1.4300667976,0.6777111405,0.3372951352
H,0,-0.1129437016,-0.7898860152,4.1201932542

H,0,-0.468204078,0.7519045514,2.2251958166
H,0,-0.1653343789,1.7189995596,3.6636662772
H,0,2.256241619,1.9260274522,3.0046521014
H,0,1.1965775456,2.6033433373,1.7711664921
H,0,3.0547889773,1.1031393821,0.8503282974
H,0,-0.1225873541,-1.4131263831,1.303958432
H,0,1.6692524127,-1.5434331858,0.5950241125
H,0,1.1652760646,-3.0649690891,1.5893163839
O,0,2.2729813553,-2.0384802495,3.8512915553
C,0,3.3397033767,-2.8617846007,3.4211272936
H,0,3.5724281297,-3.5150046568,4.2648611858
H,0,3.0615335592,-3.4818262622,2.5590285813
H,0,4.2397989958,-2.2780590131,3.1754424959

B3LYP/6-31G*
E(RB3LYP) = -375.782267609

Zero-point correction= 0.212092 (Hartree/Particle)
Thermal correction to Energy= 0.221143
Thermal correction to Enthalpy= 0.222088
Thermal correction to Gibbs Free Energy= 0.178825
Sum of electronic and ZPE= -375.570176
Sum of electronic and thermal Energies= -375.561124
Sum of electronic and thermal Enthalpies= -375.560180
Sum of electronic and thermal Free Energies= -375.603442

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.770	36.129	91.053

C,0,2.091439978,0.717034413,1.2078327718
C,0,2.319554589,-0.6986172381,1.7528632063
C,0,1.6310127999,-1.1800453397,2.9248728573
C,0,0.7513677626,-0.2339215,3.7370033495
C,0,0.3003406962,1.0118559852,2.9648519389
C,0,1.4934362156,1.6643756644,2.2595029995
B,0,0.9384745137,-1.8927303687,1.5633996509
H,0,1.3472228246,0.0785363149,4.6057446277
H,0,3.2960308143,-1.126559482,1.5418733364
H,0,1.4259868065,0.676659727,0.3382942058
H,0,-0.109566599,-0.7852524475,4.1302729939
H,0,-0.4661279773,0.7477387982,2.2254258811
H,0,-0.1650268013,1.717742614,3.6631357526
H,0,2.258918394,1.9213149191,3.0050731963

H,0,1.1990930346,2.6022393904,1.7730588057
H,0,3.0522615817,1.1020507964,0.846303268
H,0,-0.1226443396,-1.4115222999,1.2929248042
H,0,1.675885239,-1.5362187628,0.6030565358
H,0,1.1631929044,-3.0680914547,1.5784661798
O,0,2.2652021145,-2.0421727025,3.851780995
C,0,3.3341627994,-2.854887213,3.4230303299
H,0,3.5702310598,-3.5114494554,4.2645657078
H,0,3.0663237821,-3.4751891182,2.556658213
H,0,4.2355068073,-2.26927424,3.1797933927

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203608	E(Thermal)=	0.213000
E(QCISD(T))=	-374.581541	E(Empiric)=	-0.175760
DE(Plus)=	-0.021902	DE(2DF)=	-0.352207
E(Delta-G3)=	-0.510931	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.438732	G3 Energy=	-375.429341
G3 Enthalpy=	-375.428397	G3 Free Energy=	-375.472260

For Anharmonic Corrections of 6f-8

Zero-point vibrational energy 556847.2 (Joules/Mol) 133.08966 (Kcal/Mol)
Warning -- explicit consideration of 13 degrees of freedom as vibrations may cause significant error
Vibrational temperatures: 132.52 198.86 253.33 329.02 394.34
(Kelvin) 464.21 471.53 535.09 630.63 676.40
724.09 761.30 888.43 926.57 1037.54
1170.29 1179.72 1240.91 1258.80 1350.17
1355.45 1402.86 1489.19 1505.27 1543.31
1567.89 1602.90 1631.52 1679.70 1702.69
1706.23 1719.50 1730.08 1771.54 1820.22
1863.33 1893.72 1922.67 1993.16 2000.90
2010.22 2024.31 2090.70 2159.57 2180.18
2189.01 2191.94 2193.67 2212.29 2214.72
3271.73 3704.40 3853.39 4306.89 4366.54
4371.77 4390.94 4399.95 4403.17 4433.26
4443.79 4453.13 4461.37 4510.94 4582.69

Zero-point correction=	0.212092 (Hartree/Particle)
Thermal correction to Energy=	0.221144
Thermal correction to Enthalpy=	0.222088
Thermal correction to Gibbs Free Energy=	0.178825
Sum of electronic and zero-point Energies=	-375.570176

Sum of electronic and thermal Energies= -375.561124
Sum of electronic and thermal Enthalpies= -375.560180
Sum of electronic and thermal Free Energies= -375.603443

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.770	36.129	91.054

ZPE(harm) = 0.55685D+03 kJ/mol ZPE(anh)= 0.54790D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.22105D-95	0.24369D-93	
QZvib	0.79393D+02	0.23672D+03	
Energy	0.58061D+03	0.57260D+03	kJ/mol
Enthalpy	0.58309D+03	0.57508D+03	kJ/mol
Entropy	0.38928D+03	0.40151D+03	J/(mol K)
Sp.Heat(V)	0.15116D+03	0.15559D+03	J/(mol K)
Sp.Heat(P)	0.15948D+03	0.16390D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.22105D-95	0.24369D-93	
QZvib	0.79393D+02	0.23672D+03	
Energy	0.58061D+03	0.57260D+03	kJ/mol
Enthalpy	0.58309D+03	0.57508D+03	kJ/mol
Entropy	0.38928D+03	0.40151D+03	J/(mol K)
Sp.Heat(V)	0.15116D+03	0.15559D+03	J/(mol K)
Sp.Heat(P)	0.15948D+03	0.16390D+03	J/(mol K)

6f-9 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.831590433

Zero-point correction= 0.210802 (Hartree/Particle)
Thermal correction to Energy= 0.221005
Thermal correction to Enthalpy= 0.221949
Thermal correction to Gibbs Free Energy= 0.176293
Sum of electronic and ZPE= -375.620789
Sum of electronic and thermal Energies= -375.610585
Sum of electronic and thermal Enthalpies= -375.609641
Sum of electronic and thermal Free Energies= -375.655297

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.683	39.303	96.092

C,0,2.2012674349,0.626692168,1.2643223223
C,0,2.6063451648,-0.5307387886,2.1628939119
C,0,1.8378201198,-0.9140210665,3.2465779382
C,0,0.7273101996,-0.0409011256,3.8000000052
C,0,0.1461268076,0.8840343936,2.711371668
C,0,1.2507848407,1.6207565352,1.9460988078
B,0,3.7409185968,0.0456700505,3.5815925377
H,0,1.1015324809,0.5504312328,4.6423687099
H,0,3.1827698107,-1.3228752066,1.6945976939
H,0,1.7091921426,0.2003421417,0.3767325289
H,0,-0.062452997,-0.689533434,4.1921680281
H,0,-0.4463823584,0.2814536188,2.009429809
H,0,-0.5448715271,1.5946817626,3.1786039672
H,0,1.8158512441,2.2532929761,2.639845744
H,0,0.8111268826,2.2848479852,1.1930274863
H,0,3.0986866941,1.1414874636,0.9056395011
H,0,4.722699225,-0.5717278764,3.266272369
H,0,3.7163186315,1.2372911902,3.425837568
H,0,3.3880675639,-0.2550623648,4.699557044
O,0,1.955499911,-2.1961426468,3.6615179807
C,0,1.7135067458,-2.5213561983,5.0370814719
H,0,1.923322365,-3.5876143255,5.1225559732
H,0,2.3914022088,-1.9538534601,5.6821511788
H,0,0.6740348122,-2.332959025,5.3233797548

B3LYP/6-31G*
E(RB3LYP) = -375.801664931

Zero-point correction= 0.212311 (Hartree/Particle)
Thermal correction to Energy= 0.222458
Thermal correction to Enthalpy= 0.223402
Thermal correction to Gibbs Free Energy= 0.177815
Sum of electronic and ZPE= -375.589354
Sum of electronic and thermal Energies= -375.579207
Sum of electronic and thermal Enthalpies= -375.578263
Sum of electronic and thermal Free Energies= -375.623850

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.594	38.968	95.945

C,0,2.2007785682,0.6242216275,1.2642599168
C,0,2.6042070664,-0.5336958795,2.162124047
C,0,1.8354104972,-0.9186896906,3.2449420262
C,0,0.7237470354,-0.0451621028,3.7973533469
C,0,0.1472572862,0.8847231215,2.7112298132
C,0,1.2550742046,1.6196426633,1.9497972157
B,0,3.7364816189,0.046186037,3.5814381683
H,0,1.0950581631,0.5411337647,4.6448370156
H,0,3.1804784311,-1.3259481985,1.6929724225
H,0,1.7061744549,0.2017952662,0.375630008
H,0,-0.069345909,-0.6946591834,4.1838905927
H,0,-0.4462488616,0.2857833003,2.0064817125
H,0,-0.543229781,1.5960918255,3.1791768575
H,0,1.8239308575,2.2454099445,2.6469075347
H,0,0.8186049706,2.2899746569,1.1997498539
H,0,3.0993786337,1.1376404827,0.9054000483
H,0,4.7192504661,-0.5688940192,3.2631502895
H,0,3.7102187267,1.2386728784,3.4259837993
H,0,3.3867858548,-0.2537802882,4.7023183085
O,0,1.9574234685,-2.1971941751,3.6610237346
C,0,1.7177659795,-2.5155267317,5.034936658
H,0,1.9270273585,-3.582189259,5.1261943407
H,0,2.3958622446,-1.9454574785,5.6782024139
H,0,0.6787856652,-2.325882562,5.3256238758

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203818	E(Thermal)=	0.214315
E(QCISD(T))=	-374.599664	E(Empiric)=	-0.175760
DE(Plus)=	-0.021041	DE(2DF)=	-0.351288
E(Delta-G3)=	-0.511465	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.455400	G3 Energy=	-375.444903
G3 Enthalpy=	-375.443959	G3 Free Energy=	-375.490201

For Anharmonic Corrections of 6f-9

Zero-point vibrational energy 557417.4 (Joules/Mol)
133.22596 (Kcal/Mol) Warning -- explicit consideration of 14 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 113.99 152.15 240.67 276.85 286.10
(Kelvin) 366.85 407.65 450.98 482.85 500.68
593.77 656.35 697.27 807.65 926.81
1085.55 1159.86 1192.29 1206.51 1244.45

1319.73 1345.92 1393.34 1428.70 1498.48
1535.84 1579.28 1609.97 1631.49 1684.61
1697.48 1709.49 1730.69 1735.04 1739.34
1812.09 1854.23 1903.99 1928.99 1989.34
2004.17 2018.10 2046.20 2147.12 2157.66
2176.79 2189.02 2192.39 2200.80 2205.82
2333.32 3591.12 3670.64 3770.98 4334.86
4368.71 4396.04 4401.13 4415.39 4440.18
4446.94 4463.20 4474.83 4500.61 4564.03
4596.30

Zero-point correction= 0.212309 (Hartree/Particle)
Thermal correction to Energy= 0.222456
Thermal correction to Enthalpy= 0.223400
Thermal correction to Gibbs Free Energy= 0.177813
Sum of electronic and zero-point Energies= -375.589356
Sum of electronic and thermal Energies= -375.579209
Sum of electronic and thermal Enthalpies= -375.578265
Sum of electronic and thermal Free Energies= -375.623852

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.593	38.968	95.946

ZPE(harm) = 0.55742D+03 kJ/mol ZPE(anh)= 0.54621D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.62134D-95	0.39695D-93	
QZvib	0.28088D+03	0.19542D+03	
Energy	0.58406D+03	0.57106D+03	kJ/mol
Enthalpy	0.58654D+03	0.57354D+03	kJ/mol
Entropy	0.40144D+03	0.40905D+03	J/(mol K)
Sp.Heat(V)	0.16304D+03	0.15286D+03	J/(mol K)
Sp.Heat(P)	0.17136D+03	0.16118D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.62134D-95	0.39695D-93	
QZvib	0.28088D+03	0.19542D+03	
Energy	0.58406D+03	0.57106D+03	kJ/mol
Enthalpy	0.58654D+03	0.57354D+03	kJ/mol
Entropy	0.40144D+03	0.40905D+03	J/(mol K)
Sp.Heat(V)	0.16304D+03	0.15286D+03	J/(mol K)
Sp.Heat(P)	0.17136D+03	0.16118D+03	J/(mol K)

6f-10 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.826815150

Zero-point correction= 0.210512 (Hartree/Particle)
Thermal correction to Energy= 0.219674
Thermal correction to Enthalpy= 0.220619
Thermal correction to Gibbs Free Energy= 0.177114
Sum of electronic and ZPE= -375.616303
Sum of electronic and thermal Energies= -375.607141
Sum of electronic and thermal Enthalpies= -375.606197
Sum of electronic and thermal Free Energies= -375.649701

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.848	36.474	91.563

C,0,2.2126882539,0.6738991459,1.2427278233
C,0,2.3449894266,-0.6840976786,1.9510816874
C,0,1.6827876526,-0.9352830113,3.2017090805
C,0,0.7029023283,0.068197769,3.7972232555
C,0,0.2490120973,1.1315502423,2.7864252982
C,0,1.4639282444,1.7331689959,2.0708776318
B,0,1.1781257657,-1.8621933601,1.6263800596
H,0,1.2554002779,0.5607825058,4.6105191112
H,0,3.3344179327,-1.1318316793,1.9067239095
H,0,1.7010718808,0.5351563632,0.2839204396
H,0,-0.15628431,-0.4342260744,4.2518944325
H,0,-0.438537946,0.6879780413,2.0566379193
H,0,-0.3107022974,1.9074106586,3.3214453977
H,0,2.1399762682,2.1595166317,2.8259165722
H,0,1.1561441837,2.5618628034,1.4227872578
H,0,3.216305121,1.0457382755,1.0053195931
H,0,0.3007082921,-1.4327308831,0.9309034549
H,0,1.6812518371,-2.9355945382,1.4537000027
H,0,0.5905311948,-2.021754212,2.7347942624
O,0,2.3897738317,-1.7196154425,4.0763461228
C,0,1.6598634915,-2.3952207785,5.1024506107
H,0,2.3813462648,-3.0387131446,5.6068475815
H,0,1.2304876364,-1.6942600311,5.8264788318
H,0,0.8638185723,-3.0102055993,4.6628806641

B3LYP/6-31G*
E(RB3LYP) = -375.795751946

Zero-point correction= 0.211975 (Hartree/Particle)
Thermal correction to Energy= 0.221063
Thermal correction to Enthalpy= 0.222007
Thermal correction to Gibbs Free Energy= 0.178623
Sum of electronic and ZPE= -375.583777
Sum of electronic and thermal Energies= -375.574689
Sum of electronic and thermal Enthalpies= -375.573745
Sum of electronic and thermal Free Energies= -375.617129

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.719	36.072	91.310

C,0,2.2119335436,0.6730844603,1.2433562881
C,0,2.3416779495,-0.6890349889,1.945537806
C,0,1.67494485,-0.942809282,3.2001328283
C,0,0.703338332,0.0684274457,3.798463726
C,0,0.2484916,1.1291325777,2.7866580206
C,0,1.4638489868,1.7310270289,2.0731661179
B,0,1.1874537685,-1.8607229458,1.6162620707
H,0,1.2641211812,0.5607848261,4.6067762317
H,0,3.3369773726,-1.1258752738,1.9147716247
H,0,1.6995654407,0.5387652922,0.2839457143
H,0,-0.1551216794,-0.4278608089,4.2628736582
H,0,-0.4368922997,0.6823400073,2.0560493868
H,0,-0.3146258167,1.9048464154,3.3193655171
H,0,2.139315063,2.1556340132,2.8302148906
H,0,1.1571130922,2.5621591395,1.426835096
H,0,3.2153575497,1.0466512552,1.0054291495
H,0,0.2984271723,-1.4406929409,0.9281252886
H,0,1.6781448239,-2.9431774181,1.4615062153
H,0,0.5984094967,-2.0021308039,2.7379102784
O,0,2.3876606576,-1.7211568353,4.0723249267
C,0,1.6597694113,-2.3925932379,5.0976518551
H,0,2.3805134956,-3.0362186489,5.6046053687
H,0,1.2280520966,-1.6921505245,5.8221142058
H,0,0.8615299119,-3.0088937526,4.6619147346

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203850	E(Thermal)=	0.214351
E(QCISD(T))=	-374.599486	E(Empiric)=	-0.175760

DE(Plus)=	-0.020832	DE(2DF)=	-0.351756
E(Delta-G3)=	-0.511603	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.455587	G3 Energy=	-375.445087
G3 Enthalpy=	-375.444143	G3 Free Energy=	-375.490373

For Anharmonic Corrections of 6f-10

Zero-point vibrational energy 556464.6 (Joules/Mol) 132.99823 (Kcal/Mol)
Warning -- explicit consideration of 13 degrees of freedom as vibrations may cause significant error
Vibrational temperatures: 153.20 171.20 221.12 308.69 395.77
(Kelvin) 422.60 481.47 544.74 568.56 686.54
742.03 799.90 823.60 981.87 1055.81
1171.55 1196.84 1218.22 1259.52 1351.94
1352.48 1399.89 1445.03 1508.22 1551.14
1581.20 1633.59 1640.29 1667.47 1695.95
1703.70 1713.19 1722.96 1740.97 1780.09
1862.93 1889.57 1915.21 1988.70 2001.24
2011.56 2023.80 2115.04 2152.80 2176.50
2186.96 2191.12 2191.61 2199.63 2212.37
3226.06 3682.22 3825.67 4356.77 4367.73
4373.74 4395.47 4400.87 4433.55 4450.90
4457.51 4466.96 4475.31 4564.00 4567.32

Zero-point correction=	0.211946 (Hartree/Particle)
Thermal correction to Energy=	0.221100
Thermal correction to Enthalpy=	0.222044
Thermal correction to Gibbs Free Energy=	0.178511
Sum of electronic and zero-point Energies=	-375.583830
Sum of electronic and thermal Energies=	-375.574676
Sum of electronic and thermal Enthalpies=	-375.573732
Sum of electronic and thermal Free Energies=	-375.617266

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.742	36.250	91.624

ZPE(harm) = 0.55646D+03 kJ/mol ZPE(anh)= 0.54877D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.30310D-95	0.59814D-94	
QZvib	0.93294D+02	0.82525D+02	
Energy	0.58050D+03	0.57295D+03	kJ/mol

Enthalpy	0.58298D+03	0.57543D+03	kJ/mol
Entropy	0.39167D+03	0.39116D+03	J/(mol K)
Sp.Heat(V)	0.15167D+03	0.15457D+03	J/(mol K)
Sp.Heat(P)	0.15999D+03	0.16289D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.30310D-95	0.59814D-94	
QZvib	0.93294D+02	0.82525D+02	
Energy	0.58050D+03	0.57295D+03	kJ/mol
Enthalpy	0.58298D+03	0.57543D+03	kJ/mol
Entropy	0.39167D+03	0.39116D+03	J/(mol K)
Sp.Heat(V)	0.15167D+03	0.15457D+03	J/(mol K)
Sp.Heat(P)	0.15999D+03	0.16289D+03	J/(mol K)

6f-11 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.813825999

Zero-point correction= 0.210566 (Hartree/Particle)
Thermal correction to Energy= 0.219695
Thermal correction to Enthalpy= 0.220639
Thermal correction to Gibbs Free Energy= 0.177252
Sum of electronic and ZPE= -375.603260
Sum of electronic and thermal Energies= -375.594131
Sum of electronic and thermal Enthalpies= -375.593187
Sum of electronic and thermal Free Energies= -375.636574

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.861	36.529	91.316

C,0,2.2132137707,0.7031325897,1.2461687885
C,0,2.5585413921,-0.6701643407,1.834082505
C,0,1.8397550341,-1.2153070694,2.9542049713
C,0,0.7853872961,-0.3805800392,3.6736259199
C,0,0.2587202209,0.7993965398,2.8461118687
C,0,1.4220512888,1.5823153207,2.2279724234
B,0,1.3492776019,-2.0209307111,1.5479544594
H,0,1.2606890579,0.0041593683,4.586056302
H,0,3.5894685347,-0.9866887379,1.7042673908
H,0,1.6335892238,0.5775188337,0.3251842535

H,0,-0.033906055,-1.0313145621,3.9961726327
H,0,-0.4091053437,0.4432797121,2.0521714496
H,0,-0.339980921,1.4504522382,3.4933603312
H,0,2.0870033076,1.9349669799,3.028404894
H,0,1.0607388526,2.4736233339,1.7018446409
H,0,3.1501304898,1.1946092614,0.960177456
H,0,2.107433431,-1.5981446166,0.6399481616
H,0,1.7038104079,-3.1604704177,1.6166299578
H,0,0.260441809,-1.6733983491,1.1996054731
O,0,2.4949926925,-1.9934562103,3.9424266944
C,0,3.6819284562,-2.6892772101,3.6141221913
H,0,3.9189048933,-3.3040639184,4.4851122054
H,0,3.5495338136,-3.3443962236,2.7432978485
H,0,4.5251667453,-2.0059307718,3.431761181

B3LYP/6-31G*
E(RB3LYP) = -375.782267609

Zero-point correction= 0.212092 (Hartree/Particle)
Thermal correction to Energy= 0.221143
Thermal correction to Enthalpy= 0.222088
Thermal correction to Gibbs Free Energy= 0.178825
Sum of electronic and ZPE= -375.570176
Sum of electronic and thermal Energies= -375.561124
Sum of electronic and thermal Enthalpies= -375.560180
Sum of electronic and thermal Free Energies= -375.603442

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.770	36.129	91.053

C,0,2.2121076243,0.7009612153,1.2454328106
C,0,2.5577287463,-0.6738423892,1.8316259656
C,0,1.8358689942,-1.2235388973,2.9524383253
C,0,0.7884321145,-0.3808173009,3.6743651394
C,0,0.2606046347,0.7973809547,2.8468064366
C,0,1.4236377814,1.579812322,2.2287988501
B,0,1.345140273,-2.0231733297,1.5521123745
H,0,1.2704900478,0.00615912,4.5827999235
H,0,3.591358545,-0.985910043,1.7076026544
H,0,1.6295612093,0.5759912145,0.3258799638
H,0,-0.0319445567,-1.0262438352,4.0063915803
H,0,-0.4065892762,0.439410151,2.0526450881
H,0,-0.3394721417,1.4492438319,3.4928914478

H,0,2.0901849574,1.9305899197,3.0291273146
H,0,1.0632198106,2.4728429078,1.703965984
H,0,3.1480725976,1.1931901399,0.9559514502
H,0,2.1125140865,-1.5901541451,0.6483607151
H,0,1.7029881387,-3.1639065771,1.6057017104
H,0,0.2611104779,-1.6718903858,1.1885596396
O,0,2.4876785993,-1.9980322496,3.9423483553
C,0,3.6754912396,-2.6830517062,3.6154559386
H,0,3.9163458364,-3.300781299,4.4845837952
H,0,3.5537167586,-3.3372513137,2.7412096386
H,0,4.5195395016,-1.9976573052,3.4356088984

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203608	E(Thermal)=	0.212999
E(QCISD(T))=	-374.581541	E(Empiric)=	-0.175760
DE(Plus)=	-0.021902	DE(2DF)=	-0.352207
E(Delta-G3)=	-0.510931	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.438732	G3 Energy=	-375.429341
G3 Enthalpy=	-375.428397	G3 Free Energy=	-375.472260

For Anharmonic Corrections of 6f-11

Zero-point vibrational energy 556847.1 (Joules/Mol) 133.08965 (Kcal/Mol)
Warning -- explicit consideration of 13 degrees of freedom as vibrations may cause significant error
Vibrational temperatures: 132.52 198.86 253.34 329.02 394.35
(Kelvin) 464.21 471.53 535.09 630.63 676.40
724.09 761.30 888.43 926.57 1037.54
1170.29 1179.71 1240.91 1258.80 1350.17
1355.45 1402.87 1489.18 1505.27 1543.31
1567.89 1602.90 1631.52 1679.70 1702.69
1706.23 1719.50 1730.08 1771.54 1820.22
1863.33 1893.72 1922.67 1993.16 2000.90
2010.22 2024.31 2090.70 2159.57 2180.18
2189.01 2191.94 2193.67 2212.29 2214.72
3271.72 3704.40 3853.39 4306.89 4366.54
4371.77 4390.94 4399.95 4403.17 4433.26
4443.79 4453.13 4461.38 4510.94 4582.68

Zero-point correction=	0.212092 (Hartree/Particle)
Thermal correction to Energy=	0.221144
Thermal correction to Enthalpy=	0.222088
Thermal correction to Gibbs Free Energy=	0.178825

Sum of electronic and zero-point Energies= -375.570176
Sum of electronic and thermal Energies= -375.561124
Sum of electronic and thermal Enthalpies= -375.560180
Sum of electronic and thermal Free Energies= -375.603443

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.770	36.129	91.054

ZPE(harm) = 0.55685D+03 kJ/mol ZPE(anh)= 0.54789D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.22105D-95	0.24550D-93	
QZvib	0.79391D+02	0.23820D+03	
Energy	0.58061D+03	0.57260D+03	kJ/mol
Enthalpy	0.58309D+03	0.57508D+03	kJ/mol
Entropy	0.38928D+03	0.40157D+03	J/(mol K)
Sp.Heat(V)	0.15116D+03	0.15559D+03	J/(mol K)
Sp.Heat(P)	0.15948D+03	0.16391D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.22105D-95	0.24550D-93	
QZvib	0.79391D+02	0.23820D+03	
Energy	0.58061D+03	0.57260D+03	kJ/mol
Enthalpy	0.58309D+03	0.57508D+03	kJ/mol
Entropy	0.38928D+03	0.40157D+03	J/(mol K)
Sp.Heat(V)	0.15116D+03	0.15559D+03	J/(mol K)
Sp.Heat(P)	0.15948D+03	0.16391D+03	J/(mol K)

6f-12 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.812948964

Zero-point correction= 0.210512 (Hartree/Particle)
Thermal correction to Energy= 0.219634
Thermal correction to Enthalpy= 0.220578
Thermal correction to Gibbs Free Energy= 0.177212
Sum of electronic and ZPE= -375.602437
Sum of electronic and thermal Energies= -375.593315
Sum of electronic and thermal Enthalpies= -375.592371
Sum of electronic and thermal Free Energies= -375.635737

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.823	36.588	91.273

C,0,2.1787558682,0.6871328349,1.1608255853
C,0,2.704647495,-0.4977256891,1.9580296076
C,0,2.1063562193,-0.9047342983,3.1993152387
C,0,0.8852224011,-0.1597851417,3.7560571824
C,0,0.2274892662,0.7913835463,2.7409933422
C,0,1.2681159498,1.6168355582,1.9737309982
B,0,3.6162593257,-0.1815597301,3.5152407768
H,0,1.1655499839,0.3947484166,4.6563683956
H,0,3.1803068645,-1.2677259958,1.3561115558
H,0,1.5967204149,0.2520330063,0.3353717571
H,0,0.1676164058,-0.9257437652,4.065143332
H,0,-0.3604130923,0.2067778738,2.0188223865
H,0,-0.4787448297,1.4491769534,3.2603775205
H,0,1.8658596357,2.2138429206,2.6727048547
H,0,0.7775707703,2.3214977837,1.2923523202
H,0,3.0074262972,1.2402994752,0.7035457572
H,0,3.4819553285,0.8848332905,4.0322579947
H,0,4.3800954817,-1.0132941034,3.9073541694
H,0,4.1086790915,0.071578657,2.3881701427
O,0,1.9663115544,-2.2763971086,3.5355326809
C,0,2.8535051882,-3.2280036069,2.9799125683
H,0,2.6311483922,-4.1718881738,3.4822950236
H,0,2.6918907009,-3.3630784061,1.8997313411
H,0,3.9040832869,-2.9675942971,3.1609954686

B3LYP/6-31G*
E(RB3LYP) = -375.781348492

Zero-point correction= 0.211991 (Hartree/Particle)
Thermal correction to Energy= 0.221045
Thermal correction to Enthalpy= 0.221990
Thermal correction to Gibbs Free Energy= 0.178717
Sum of electronic and ZPE= -375.569358
Sum of electronic and thermal Energies= -375.560303
Sum of electronic and thermal Enthalpies= -375.559359
Sum of electronic and thermal Free Energies= -375.602632

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.708	36.203	91.075

C,0,2.1773590985,0.6826321445,1.159256837
C,0,2.7100017265,-0.4971416821,1.9602452949
C,0,2.1114507736,-0.9065720866,3.2054621462
C,0,0.8843926247,-0.162663065,3.7547641206
C,0,0.2306782663,0.7917029072,2.7406604261
C,0,1.2733537769,1.6150031295,1.9751881542
B,0,3.6106533903,-0.1824040863,3.5242326026
H,0,1.1563810511,0.389049274,4.6597699319
H,0,3.1850422958,-1.2684715632,1.3583558974
H,0,1.5889655909,0.2433417351,0.3401172681
H,0,0.1647839379,-0.9306354525,4.0555578864
H,0,-0.3576939138,0.2099902359,2.0160150492
H,0,-0.4755747857,1.4507691273,3.259490338
H,0,1.8755794828,2.2072442051,2.6749069859
H,0,0.7850940551,2.3242527413,1.296094488
H,0,3.0020160728,1.2343345152,0.6918783829
H,0,3.4823809766,0.8895297951,4.0346009493
H,0,4.3902540128,-1.0068547862,3.904222977
H,0,4.0921881776,0.0770143983,2.3869207182
O,0,1.9680545162,-2.2753612707,3.5413794686
C,0,2.8494874226,-3.2214528605,2.9801360366
H,0,2.6309789549,-4.1691392724,3.4792406102
H,0,2.6873253492,-3.356522791,1.8984396959
H,0,3.9032551463,-2.9650352919,3.1543037349

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203511	E(Thermal)=	0.212907
E(QCISD(T))=	-374.580068	E(Empiric)=	-0.175760
DE(Plus)=	-0.022068	DE(2DF)=	-0.352642
E(Delta-G3)=	-0.510567	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.437594	G3 Energy=	-375.428199
G3 Enthalpy=	-375.427254	G3 Free Energy=	-375.471129

For Anharmonic Corrections of 6f-12

Zero-point correction=	0.211992 (Hartree/Particle)
Thermal correction to Energy=	0.221046
Thermal correction to Enthalpy=	0.221990
Thermal correction to Gibbs Free Energy=	0.178718
Sum of electronic and zero-point Energies=	-375.569357

Sum of electronic and thermal Energies= -375.560302
Sum of electronic and thermal Enthalpies= -375.559358
Sum of electronic and thermal Free Energies= -375.602631

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.708	36.203	91.074

6f-13 Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.819390997

Zero-point correction= 0.210504 (Hartree/Particle)
Thermal correction to Energy= 0.219687
Thermal correction to Enthalpy= 0.220631
Thermal correction to Gibbs Free Energy= 0.177229
Sum of electronic and ZPE= -375.608887
Sum of electronic and thermal Energies= -375.599704
Sum of electronic and thermal Enthalpies= -375.598760
Sum of electronic and thermal Free Energies= -375.642162

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	137.856	36.717	91.347

C,0,2.1030342843,0.4793077414,1.2021824598
C,0,2.4709070619,-0.670974868,2.1379469501
C,0,1.7939849899,-0.8896183291,3.3711869674
C,0,0.751092778,0.1054105135,3.8782704138
C,0,0.2119392622,1.0384698313,2.7824632253
C,0,1.3579066846,1.605703534,1.9382136864
B,0,1.2629805128,-2.054957825,2.2252856825
H,0,1.2482429454,0.7094225395,4.6509231016
H,0,3.4973503438,-1.0269166437,2.1080786224
H,0,1.4802847457,0.1098451341,0.3806315501
H,0,-0.0779365921,-0.4181563365,4.3660682196
H,0,-0.4872551306,0.4948068802,2.1357116198
H,0,-0.3570377378,1.8487885839,3.2526958368
H,0,2.0565336554,2.1475861118,2.5903022251
H,0,0.9820535452,2.3298049971,1.2061137243
H,0,3.0250272224,0.8592105083,0.7481092333
H,0,0.1634242847,-1.7930931672,1.8316271075

H,0,2.0006748817,-1.9640010347,1.2266817463
H,0,1.5785106982,-3.1255323923,2.65289295
O,0,2.6405071073,-1.4080018192,4.3747721747
C,0,2.0158721941,-2.2208015256,5.3606251189
H,0,2.8162257115,-2.576859943,6.0128124513
H,0,1.2952672943,-1.6525781206,5.9632627104
H,0,1.5082792569,-3.0785753704,4.9020772222

B3LYP/6-31G*
E(RB3LYP) = -375.787990685

Zero-point correction= 0.212022 (Hartree/Particle)
Thermal correction to Energy= 0.221114
Thermal correction to Enthalpy= 0.222059
Thermal correction to Gibbs Free Energy= 0.178831
Sum of electronic and ZPE= -375.575969
Sum of electronic and thermal Energies= -375.566876
Sum of electronic and thermal Enthalpies= -375.565932
Sum of electronic and thermal Free Energies= -375.609160

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	138.751	36.305	90.980

C,0,2.0993709858,0.4757894639,1.2010769425
C,0,2.4686859936,-0.6733123151,2.1389563534
C,0,1.7879125228,-0.8942200466,3.3745039407
C,0,0.7528242114,0.1102863757,3.8802728439
C,0,0.2131018993,1.0403271205,2.7833626385
C,0,1.3586986031,1.6044318969,1.9372303751
B,0,1.2601623285,-2.0533398552,2.2370150688
H,0,1.2568538957,0.7150987316,4.6483237228
H,0,3.4989997492,-1.0198854082,2.1168803261
H,0,1.4712573118,0.1044372302,0.3840765066
H,0,-0.0771361421,-0.4051512744,4.376488896
H,0,-0.4863643284,0.4945148245,2.1379642328
H,0,-0.3562629755,1.8527294949,3.2506940006
H,0,2.0600028889,2.1451489165,2.5879397472
H,0,0.9838608876,2.3294052901,1.2047268268
H,0,3.0190867208,0.8537842444,0.7397941776
H,0,0.1665258139,-1.7945816208,1.8223678611
H,0,2.0104782433,-1.9524737863,1.2409141871
H,0,1.5788360919,-3.1303461405,2.6495268116

O,0,2.6382787307,-1.4040776208,4.3764887801
C,0,2.0161751796,-2.2230759231,5.3525188869
H,0,2.8140722694,-2.5691346359,6.014785966
H,0,1.2794125305,-1.6686243223,5.9505225564
H,0,1.5230365882,-3.0894416401,4.8925033513

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.203541	E(Thermal)=	0.212975
E(QCISD(T))=	-374.587761	E(Empiric)=	-0.175760
DE(Plus)=	-0.022222	DE(2DF)=	-0.351502
E(Delta-G3)=	-0.510424	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.444129	G3 Energy=	-375.434694
G3 Enthalpy=	-375.433750	G3 Free Energy=	-375.477582

For Anharmonic Corrections of 6f-13

Zero-point vibrational energy 556662.1 (Joules/Mol) 133.04543 (Kcal/Mol)
Warning -- explicit consideration of 13 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 179.99 190.91 245.85 288.48 386.68
(Kelvin) 454.07 486.04 543.58 587.94 684.70
723.02 758.40 871.42 911.49 1018.26
1170.40 1179.17 1236.94 1256.78 1350.07
1358.29 1402.96 1491.09 1505.33 1546.46
1560.41 1596.75 1629.87 1677.10 1697.88
1710.87 1717.61 1726.27 1766.11 1787.18
1863.15 1886.35 1914.24 1994.13 1998.63
2002.73 2026.58 2120.54 2159.04 2180.56
2185.48 2190.74 2195.72 2213.04 2215.91
3324.47 3697.58 3843.33 4347.26 4356.86
4369.84 4393.61 4404.83 4428.79 4435.73
4438.26 4452.22 4464.63 4515.56 4583.73

Zero-point correction= 0.212021 (Hartree/Particle)
Thermal correction to Energy= 0.221114
Thermal correction to Enthalpy= 0.222058
Thermal correction to Gibbs Free Energy= 0.178831
Sum of electronic and zero-point Energies= -375.575969
Sum of electronic and thermal Energies= -375.566876
Sum of electronic and thermal Enthalpies= -375.565932
Sum of electronic and thermal Free Energies= -375.609160

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.751	36.306	90.980

ZPE(harm) = 0.55666D+03 kJ/mol ZPE(anh)= 0.54804D+03 kJ/mol

Input values of T(K) and P(atm): 298.15 1.00

	Harmonic value	SPT anharmonic value	
Qvib	0.21954D-95	0.83758D-94	
QZvib	0.73178D+02	0.86052D+02	
Energy	0.58054D+03	0.57246D+03	kJ/mol
Enthalpy	0.58301D+03	0.57494D+03	kJ/mol
Entropy	0.38898D+03	0.39217D+03	J/(mol K)
Sp.Heat(V)	0.15190D+03	0.15610D+03	J/(mol K)
Sp.Heat(P)	0.16022D+03	0.16442D+03	J/(mol K)

T = 298.15 K; P = 1.00 atm

	Harmonic value	SPT anharmonic value	
Qvib	0.21954D-95	0.83758D-94	
QZvib	0.73178D+02	0.86052D+02	
Energy	0.58054D+03	0.57246D+03	kJ/mol
Enthalpy	0.58301D+03	0.57494D+03	kJ/mol
Entropy	0.38898D+03	0.39217D+03	J/(mol K)
Sp.Heat(V)	0.15190D+03	0.15610D+03	J/(mol K)
Sp.Heat(P)	0.16022D+03	0.16442D+03	J/(mol K)

6f-14 Transition State

B3LYP/6-31+G**

E(RB3LYP) = -375.818386630

Zero-point correction= 0.210418 (Hartree/Particle)
Thermal correction to Energy= 0.219630
Thermal correction to Enthalpy= 0.220575
Thermal correction to Gibbs Free Energy= 0.177116
Sum of electronic and ZPE= -375.607968
Sum of electronic and thermal Energies= -375.598756
Sum of electronic and thermal Enthalpies= -375.597812
Sum of electronic and thermal Free Energies= -375.641270

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	137.820	36.789	91.466

C,0,0.1432411047,0.926069561,2.6047996614
C,0,1.2981518195,1.6229512014,1.8751516946
C,0,2.218647916,0.5763888305,1.2323969132
C,0,2.5949085234,-0.5511364279,2.1752691568
C,0,1.8753378696,-0.8127825562,3.3745173404
C,0,0.6388076895,0.0220376356,3.750755726
B,0,3.4060694384,-0.1075444035,3.7622266334
O,0,1.7800719129,-2.18781711,3.6762800305
C,0,1.7420489171,-2.5188942909,5.0590204124
H,0,0.8406729674,0.6279017343,4.6394163311
H,0,3.0743466518,-1.4157377638,1.7224143285
H,0,1.6872341343,0.0974936728,0.3967645278
H,0,-0.1575989777,-0.6813904172,4.0171029583
H,0,-0.4125168707,0.3162197676,1.878649966
H,0,-0.5636978858,1.6638873604,3.0012370865
H,0,1.8668044184,2.2461014432,2.57500901
H,0,0.9122330794,2.28955959,1.0954578325
H,0,3.1156710233,1.0398599645,0.8074216628
H,0,4.0540563417,-0.0071397217,2.7048273949
H,0,3.2605515072,1.0066327404,4.1669930449
H,0,4.0374869526,-0.9359450229,4.3481613501
H,0,1.6574168772,-3.6064990085,5.1098533877
H,0,2.6588594454,-2.196108292,5.5675272781
H,0,0.8748191444,-2.0716644871,5.563225272

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205428	E(Thermal)=	0.215616
E(QCISD(T))=	-374.621019	E(Empiric)=	-0.175760
DE(Plus)=	-0.021413	DE(2DF)=	-0.350600
E(Delta-G3)=	-0.510393	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.473758	G3 Energy=	-375.463569
G3 Enthalpy=	-375.462625	G3 Free Energy=	-375.507998

6f-15 Product
B3LYP/6-31+G**
E(RB3LYP) = -375.849446305

Zero-point correction= 0.212388 (Hartree/Particle)
Thermal correction to Energy= 0.222318
Thermal correction to Enthalpy= 0.223263
Thermal correction to Gibbs Free Energy= 0.178311
Sum of electronic and ZPE= -375.637059
Sum of electronic and thermal Energies= -375.627128
Sum of electronic and thermal Enthalpies= -375.626184

Sum of electronic and thermal Free Energies= -375.671135

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.507	38.614	94.608

C,0,2.0308131966,0.7948843832,0.9698093307
C,0,3.0141393822,0.1917523963,1.9842124025
C,0,2.3000340641,-0.6038521777,3.1065965404
C,0,1.2529312291,0.3303917888,3.8000302876
C,0,0.2634111741,0.9311548531,2.7832022
C,0,0.991285152,1.6888537248,1.6633925989
B,0,3.1982750279,-1.0312284569,4.3195802206
H,0,1.7815330555,1.1446346192,4.312547377
H,0,3.7451578569,-0.4460419126,1.4722714167
H,0,1.5157948465,-0.0151792557,0.438503837
H,0,0.7023987461,-0.2382159401,4.5589158311
H,0,-0.3354617636,0.1209425393,2.3529873319
H,0,-0.4270393122,1.6000625873,3.3119032139
H,0,1.4969983545,2.5696068337,2.0873193261
H,0,0.2665889537,2.0673277284,0.9319072601
H,0,2.5852482713,1.3687137409,0.216854937
H,0,3.5952299732,0.9938002801,2.4584072528
H,0,3.0294301974,-2.0737479363,4.8776513586
H,0,3.9977313061,-0.2583011146,4.7599761696
O,0,1.5041631613,-1.6850100543,2.5592369385
C,0,2.2340798231,-2.7533253086,1.9884429358
H,0,1.5120145729,-3.540762863,1.7569998085
H,0,2.7436873886,-2.4634248211,1.0579296299
H,0,2.9812833428,-3.1594406344,2.687720795

B3LYP/6-31G*
E(RB3LYP) = -375.819155618

Zero-point correction= 0.213989 (Hartree/Particle)
Thermal correction to Energy= 0.223828
Thermal correction to Enthalpy= 0.224772
Thermal correction to Gibbs Free Energy= 0.180045
Sum of electronic and ZPE= -375.605166
Sum of electronic and thermal Energies= -375.595328
Sum of electronic and thermal Enthalpies= -375.594384
Sum of electronic and thermal Free Energies= -375.639111

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.454	38.261	94.136

C,0,2.0318689177,0.7890245637,0.9706131548
C,0,3.0191092762,0.1958409074,1.9862980964
C,0,2.3044655486,-0.6026737296,3.1057380062
C,0,1.2599459954,0.3344501519,3.8026262366
C,0,0.2664263818,0.9248502808,2.7846361274
C,0,0.9894350527,1.6808483282,1.6612120351
B,0,3.1940465181,-1.0354924661,4.3221199603
H,0,1.7889937344,1.1518417357,4.3101113492
H,0,3.7529559267,-0.4399396983,1.4748113971
H,0,1.5201881464,-0.0284809178,0.4472461123
H,0,0.7125449209,-0.2313314386,4.5665253178
H,0,-0.3257862239,0.1073063684,2.3589068561
H,0,-0.4296079463,1.5917056464,3.3095521835
H,0,1.4915435781,2.5657416551,2.0814643448
H,0,0.2620083595,2.0538218756,0.9288483871
H,0,2.5807015616,1.3609081694,0.2115127096
H,0,3.5966115421,1.0017306435,2.4592325614
H,0,3.008124143,-2.0740222515,4.8851855635
H,0,4.0026586709,-0.273087583,4.7670348
O,0,1.5026325111,-1.6736005854,2.5569769486
C,0,2.2283490357,-2.7388113724,1.9836290291
H,0,1.5044627738,-3.5247613967,1.7487789131
H,0,2.7417063066,-2.4512366901,1.0533969451
H,0,2.9763432688,-3.1510371967,2.679941965

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205430 E	(Thermal)=	0.215617
E(QCISD(T))=	-374.621021	E(Empiric)=	-0.175760
DE(Plus)=	-0.021413	DE(2DF)=	-0.350603
E(Delta-G3)=	-0.510393	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.473759	G3 Energy=	-375.463572
G3 Enthalpy=	-375.462627	G3 Free Energy=	-375.507996

6f-16 Product
B3LYP/6-31+G**
E(RB3LYP) = -375.847788682

Zero-point correction= 0.212324 (Hartree/Particle)

Thermal correction to Energy= 0.222268
Thermal correction to Enthalpy= 0.223212
Thermal correction to Gibbs Free Energy= 0.178315
Sum of electronic and ZPE= -375.635465
Sum of electronic and thermal Energies= -375.625521
Sum of electronic and thermal Enthalpies= -375.624577
Sum of electronic and thermal Free Energies= -375.669474

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.475	38.705	94.494

C,0,1.9713752005,0.7089985832,0.9123112094
C,0,2.9525680082,0.2387137472,1.9987681463
C,0,2.2727563348,-0.4461839721,3.2107426677
C,0,1.1032598577,0.4560321251,3.7307318676
C,0,0.1447909182,0.9666409396,2.642631532
C,0,0.8978434453,1.6418161147,1.4881301001
O,0,3.1861682089,-0.4783711464,4.3386686418
H,0,1.5992419579,1.303014639,4.2242602916
H,0,3.7019201481,-0.4262239977,1.5523393315
H,0,1.4875723039,-0.1567299342,0.4415360131
H,0,0.5490215572,-0.0644106446,4.5232866559
H,0,-0.4563443458,0.1387170862,2.2453653059
H,0,-0.5632098585,1.669950645,3.0979865272
H,0,1.3761364473,2.5618759974,1.8541523891
H,0,0.1939400192,1.9441957692,0.7031260001
H,0,2.5328401987,1.2190136941,0.1198356348
H,0,3.4998061753,1.1075939259,2.3923727048
B,0,1.5746901845,-1.8296190679,2.9614566764
H,0,1.6440282637,-2.6963494819,3.7798747882
H,0,0.8874057015,-2.0068648877,2.0010842252
C,0,4.3048340402,-1.3354068801,4.2036975241
H,0,4.8152760348,-1.3390810214,5.1702418968
H,0,4.0060269965,-2.3675597301,3.9641792918
H,0,5.0111632016,-0.9849905025,3.4375685783

B3LYP/6-31G*
E(RB3LYP) = -375.816834892

Zero-point correction= 0.213829 (Hartree/Particle)
Thermal correction to Energy= 0.223704
Thermal correction to Enthalpy= 0.224648
Thermal correction to Gibbs Free Energy= 0.179895

Sum of electronic and ZPE= -375.603006
Sum of electronic and thermal Energies= -375.593131
Sum of electronic and thermal Enthalpies= -375.592187
Sum of electronic and thermal Free Energies= -375.636940

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.376	38.376	94.191

C,0,1.9734376954,0.7081053497,0.9145336312
C,0,2.9537395965,0.2395641867,2.001476216
C,0,2.2736257051,-0.4476186113,3.2118944843
C,0,1.1058563003,0.4583437719,3.7317311099
C,0,0.1463970079,0.9647702752,2.6437077132
C,0,0.898969498,1.639701877,1.489336856
O,0,3.1808303514,-0.4810415639,4.3394237424
H,0,1.6042393243,1.3072794547,4.2200986076
H,0,3.7055943324,-0.4239357147,1.5556391275
H,0,1.4908732753,-0.1593613979,0.4447551761
H,0,0.5523380786,-0.0579933967,4.5280362481
H,0,-0.4518970288,0.1335138856,2.2478509471
H,0,-0.5649052093,1.6669819171,3.0968721654
H,0,1.3764260143,2.5604162632,1.8557478656
H,0,0.1949309247,1.942122227,0.703826316
H,0,2.5337871736,1.2181392251,0.1205919896
H,0,3.5001842588,1.1085354987,2.3968641834
B,0,1.5726762312,-1.8297778765,2.9623129212
H,0,1.6275440904,-2.6912190396,3.789471642
H,0,0.8952102831,-2.0176753198,1.9951220916
C,0,4.2985932055,-1.3309924368,4.1977742037
H,0,4.8091768562,-1.3439766369,5.1652685704
H,0,4.0068002915,-2.3635730769,3.9461803744
H,0,5.0086827435,-0.9755368609,3.4358318172

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205276	E(Thermal)=	0.215500
E(QCISD(T))=	-374.618042	E(Empiric)=	-0.175760
DE(Plus)=	-0.021588	DE(2DF)=	-0.350281
E(Delta-G3)=	-0.511026	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.471421	G3 Energy=	-375.461197
G3 Enthalpy=	-375.460253	G3 Free Energy=	-375.505649

6f-18 Product
B3LYP/6-31G**
E(RB3LYP) = -375.847787597

Zero-point correction= 0.212324 (Hartree/Particle)
Thermal correction to Energy= 0.222269
Thermal correction to Enthalpy= 0.223213
Thermal correction to Gibbs Free Energy= 0.178312
Sum of electronic and ZPE= -375.635464
Sum of electronic and thermal Energies= -375.625519
Sum of electronic and thermal Enthalpies= -375.624575
Sum of electronic and thermal Free Energies= -375.669476

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.476	38.704	94.502

C,0,2.0342659202,0.523350086,1.0278085401
C,0,2.8338181514,-0.1564139743,2.1511428141
C,0,1.9756214078,-0.6678078008,3.3570355508
C,0,1.0114495318,0.4549624515,3.8164490698
C,0,0.202042545,1.0929693388,2.6756249713
C,0,1.1171463358,1.6296192324,1.5670902382
O,0,2.9707659325,-0.9173177084,4.3834123088
H,0,1.6308471264,1.226781088,4.2960661129
H,0,3.4470623098,-0.9747552826,1.7506067482
H,0,1.4280729615,-0.2169215002,0.4900577031
H,0,0.3264172863,0.0810577608,4.58715559
H,0,-0.4932158757,0.3576038747,2.2501506064
H,0,-0.4152057547,1.9025193988,3.0843166805
H,0,1.7315876619,2.4480901987,1.9693712716
H,0,0.5197447645,2.0562486043,0.7520861982
H,0,2.7377130761,0.9361071792,0.2942794618
H,0,3.5437826735,0.5559465112,2.5931847167
B,0,1.3331735415,-1.989465375,2.806064264
H,0,1.8153824802,-3.0501286878,3.0679625087
H,0,0.4154005511,-1.954451147,2.0428473188
C,0,2.4932060414,-1.5122658525,5.5758818696
H,0,3.371691738,-1.7504824572,6.1810776059
H,0,1.8460339941,-0.8352315253,6.1516627349
H,0,1.9431465996,-2.4452954132,5.3787641155

B3LYP/6-31G*
E(RB3LYP) = -375.816834137

Zero-point correction= 0.213829 (Hartree/Particle)
Thermal correction to Energy= 0.223705
Thermal correction to Enthalpy= 0.224649
Thermal correction to Gibbs Free Energy= 0.179892
Sum of electronic and ZPE= -375.603005
Sum of electronic and thermal Energies= -375.593129
Sum of electronic and thermal Enthalpies= -375.592185
Sum of electronic and thermal Free Energies= -375.636943

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.377	38.376	94.201

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205276	E(Thermal)=	0.215499
E(QCISD(T))=	-374.618044	E(Empiric)=	-0.175760
DE(Plus)=	-0.021588	DE(2DF)=	-0.350281
E(Delta-G3)=	-0.511027	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.471424	G3 Energy=	-375.461200
G3 Enthalpy=	-375.460256	G3 Free Energy=	-375.505651

6f-19 Product
B3LYP/6-31G**
E(RB3LYP) = -375.854976370

Zero-point correction= 0.212037 (Hartree/Particle)
Thermal correction to Energy= 0.221947
Thermal correction to Enthalpy= 0.222892
Thermal correction to Gibbs Free Energy= 0.177656
Sum of electronic and ZPE= -375.642939
Sum of electronic and thermal Energies= -375.633029
Sum of electronic and thermal Enthalpies= -375.632085
Sum of electronic and thermal Free Energies= -375.677320

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.274	38.143	95.206

C,0,2.0853964825,0.5243872294,1.0914837424
C,0,2.9730388577,-0.026410609,2.2144995017
C,0,2.0991802939,-0.6560623202,3.3243808847
C,0,1.0786148576,0.3628573311,3.8771956266
C,0,0.1871784299,0.8979090235,2.7440044946
C,0,1.0280558369,1.5116026412,1.6129824989
H,0,2.7770872355,-0.9682634016,4.1547277892
H,0,1.6059171409,1.2046981918,4.3437281407
H,0,3.6502938232,-0.7931419171,1.8048652671
H,0,1.5898160607,-0.3280801444,0.6042247644
H,0,0.46536671,-0.1079212664,4.6544692349
H,0,-0.4190931106,0.0704429883,2.3435690573
H,0,-0.5191789095,1.640179939,3.1356273371
H,0,1.5353041742,2.4097912374,1.9855225521
H,0,0.3805572463,1.8311167021,0.7872179348
H,0,2.720372241,1.0028458582,0.3376312842
O,0,3.7679483063,1.0725467764,2.6811844306
B,0,1.5603542214,-2.0828012218,3.0045381534
H,0,0.5860943646,-2.507783425,3.5553279007
H,0,2.1683674765,-2.8157430127,2.2768138056
C,0,4.8863651935,0.7070955025,3.4649439112
H,0,5.4520035854,1.6216094918,3.659088527
H,0,4.5972870888,0.2644733807,4.4302117912
H,0,5.5331743934,-0.0074889752,2.9320213695

B3LYP/6-31G*
E(RB3LYP) = -375.824081400

Zero-point correction= 0.213638 (Hartree/Particle)
Thermal correction to Energy= 0.223467
Thermal correction to Enthalpy= 0.224411
Thermal correction to Gibbs Free Energy= 0.179370
Sum of electronic and ZPE= -375.610443
Sum of electronic and thermal Energies= -375.600615
Sum of electronic and thermal Enthalpies= -375.599670
Sum of electronic and thermal Free Energies= -375.644711

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.228	37.772	94.796

C,0,2.0857797907,0.5118345168,1.0916643013
C,0,2.9760328405,-0.0317691176,2.2164434376
C,0,2.1033508363,-0.663967563,3.3269197263

C,0,1.0910917012,0.3615365698,3.8811941007
C,0,0.1977498456,0.8985987409,2.7514598036
C,0,1.035729283,1.5049915826,1.6149966829
H,0,2.7842082142,-0.9747288704,4.1544376955
H,0,1.6277142242,1.20073827,4.3422378741
H,0,3.6589836601,-0.7959507255,1.809929833
H,0,1.5863658036,-0.3418684192,0.6095309896
H,0,0.4779947425,-0.1018946273,4.6635841397
H,0,-0.4145339344,0.0728404638,2.3556478631
H,0,-0.5039623087,1.645340405,3.1443654534
H,0,1.5519245003,2.3998854422,1.9837449309
H,0,0.3858419324,1.8282444233,0.7919663225
H,0,2.7192702035,0.9863949299,0.3334660148
O,0,3.7535385333,1.0749758268,2.6811261473
B,0,1.5460407948,-2.0813931649,2.9900812943
H,0,0.5544522339,-2.496288689,3.5197413041
H,0,2.1537454922,-2.8198154279,2.2658003723
C,0,4.8712099686,0.7215314532,3.4644559274
H,0,5.4245074233,1.6430233402,3.6661029441
H,0,4.5898269199,0.2679638793,4.428042866
H,0,5.5326392991,0.0176367612,2.9333199756

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205096	E(Thermal)=	0.215261
E(QCISD(T))=	-374.625105	E(Empiric)=	-0.175760
DE(Plus)=	-0.021400	DE(2DF)=	-0.350479
E(Delta-G3)=	-0.510912	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.478560	G3 Energy=	-375.468395
G3 Enthalpy=	-375.467451	G3 Free Energy=	-375.513116

6f-20 Product
B3LYP/6-31G**
E(RB3LYP) = -375.856105180

Zero-point correction= 0.212794 (Hartree/Particle)
Thermal correction to Energy= 0.222462
Thermal correction to Enthalpy= 0.223406
Thermal correction to Gibbs Free Energy= 0.178930
Sum of electronic and ZPE= -375.643311
Sum of electronic and thermal Energies= -375.633644

Sum of electronic and thermal Enthalpies= -375.632699
Sum of electronic and thermal Free Energies= -375.677175

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.597	37.810	93.606

C,0,2.0566850953,0.4481147024,1.0693738787
C,0,2.0566850953,0.4481147024,1.0693738787
C,0,2.9825964319,-0.0244034848,2.1891650139
C,0,2.1937499548,-0.6179887585,3.3872088816
C,0,1.1663816534,0.4427279656,3.8941005105
C,0,0.2321801787,0.918311871,2.7696378597
C,0,1.0274718695,1.4686026967,1.5771699153
B,0,3.0954190195,-1.0197439839,4.6067968096
H,0,1.7066522004,1.3070219282,4.3058102276
O,0,3.8645969604,-0.9903952771,1.6119925302
H,0,1.5432899628,-0.4303882562,0.6563951849
H,0,0.5730509928,0.0275986265,4.7180789656
H,0,-0.3907464143,0.0763411673,2.4368442924
H,0,-0.4522777163,1.6835844606,3.1569553748
H,0,1.5445600998,2.3899582915,1.8823252647
H,0,0.3495546888,1.7496723846,0.7625190383
H,0,2.661437182,0.873939718,0.2606630241
H,0,3.5830346254,0.829691011,2.5519029864
H,0,2.9959385771,-2.0817049501,5.1511322884
H,0,3.8354032943,-0.2060829579,5.0851133708
H,0,1.626605275,-1.4776051978,3.0018302418
C,0,4.928937559,-1.377251071,2.4446747507
H,0,5.5217799964,-2.1147321753,1.8984780506
H,0,5.5648664812,-0.5259920123,2.7268869146
H,0,4.5745980321,-1.8690536984,3.3769456247

B3LYP/6-31G*
E(RB3LYP) = -375.825279617

Zero-point correction= 0.214327 (Hartree/Particle)
Thermal correction to Energy= 0.223900
Thermal correction to Enthalpy= 0.224844
Thermal correction to Gibbs Free Energy= 0.180570
Sum of electronic and ZPE= -375.610953
Sum of electronic and thermal Energies= -375.601379
Sum of electronic and thermal Enthalpies= -375.600435
Sum of electronic and thermal Free Energies= -375.644709

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.499	37.441	93.183

C,0,2.0570107079,0.4455403751,1.0708562468
C,0,2.983088385,-0.0274754064,2.1910478788
C,0,2.1905529562,-0.6191286725,3.3895421892
C,0,1.1660430831,0.4439158037,3.8938638001
C,0,0.2336303567,0.9190301542,2.7685598163
C,0,1.0302843948,1.468083493,1.576987493
B,0,3.0970817237,-1.0265203455,4.6038939873
H,0,1.7088969575,1.307516727,4.304345565
O,0,3.8574109473,-0.9948321914,1.6145234123
H,0,1.5421447449,-0.4334501616,0.6597716723
H,0,0.5716405095,0.0324820264,4.7195425258
H,0,-0.3893074426,0.0767403576,2.4353870857
H,0,-0.4521766379,1.6847204621,3.1539371761
H,0,1.5500907123,2.3879232006,1.8831922755
H,0,0.3532316363,1.7519118503,0.7618900324
H,0,2.6626323776,0.8675922661,0.260113538
H,0,3.5820530165,0.8273602121,2.5552502643
H,0,3.0080929468,-2.0961285774,5.1370297638
H,0,3.8303852686,-0.2113344008,5.0921152898
H,0,1.6226826588,-1.4771085082,3.0008818453
C,0,4.9236793838,-1.3689043496,2.4425821218
H,0,5.5126435978,-2.1175928034,1.9057054479
H,0,5.5661364215,-0.5167343981,2.7114867632
H,0,4.5778372936,-1.8433841134,3.3894948095

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205754	E(Thermal)=	0.215670
E(QCISD(T))=	-374.625513	E(Empiric)=	-0.175760
DE(Plus)=	-0.021865	DE(2DF)=	-0.351128
E(Delta-G3)=	-0.510457	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.478970	G3 Energy=	-375.469054
G3 Enthalpy=	-375.468110	G3 Free Energy=	-375.513005

6f-21 Product
B3LYP/6-31+G**
E(RB3LYP) = -375.850688776

Zero-point correction= 0.214542 (Hartree/Particle)

Thermal correction to Energy= 0.223636
Thermal correction to Enthalpy= 0.224580
Thermal correction to Gibbs Free Energy= 0.181409
Sum of electronic and ZPE= -375.636147
Sum of electronic and thermal Energies= -375.627053
Sum of electronic and thermal Enthalpies= -375.626109
Sum of electronic and thermal Free Energies= -375.669280

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.334	36.678	90.861

C,0,2.3315527423,0.7279555643,1.5886729509
C,0,2.7871044936,-0.255970396,2.6634237434
C,0,1.7611701002,-0.9100377605,3.5955322757
C,0,0.4538771948,-0.104758022,3.764637968
C,0,-0.0391976407,0.5461956634,2.4636164162
C,0,1.0333594595,1.4917989941,1.9025133344
B,0,2.8445741173,-0.8122782083,4.8098952548
H,0,0.5962452032,0.6880925388,4.5121248092
H,0,3.4392860924,-1.0069896404,2.2112972836
H,0,2.1530194757,0.1086655007,0.6985531823
H,0,-0.3180225284,-0.764391979,4.1791165126
H,0,-0.2725300519,-0.227777664,1.717106887
H,0,-0.9690774528,1.1001278262,2.6423364401
H,0,1.2201509708,2.2927870399,2.6301235898
H,0,0.6816732798,1.9835429316,0.987507613
H,0,3.1494067226,1.4057501217,1.313217582
O,0,3.6977068024,0.2887974026,3.750150065
H,0,2.5603841308,-0.179302471,5.7957800083
H,0,3.6149628935,-1.7225392042,4.9627726131
H,0,1.5300717617,-1.9257130204,3.2523557673
C,0,3.7291217292,1.6824691371,4.0807255698
H,0,4.4249470887,1.773133188,4.9166618631
H,0,4.1037527709,2.2577270108,3.2301811871
H,0,2.7448606446,2.0484734469,4.3869290831

B3LYP/6-31G*
E(RB3LYP) = -375.821348994

Zero-point correction= 0.216123 (Hartree/Particle)
Thermal correction to Energy= 0.225150
Thermal correction to Enthalpy= 0.226094
Thermal correction to Gibbs Free Energy= 0.183035

Sum of electronic and ZPE= -375.605226
Sum of electronic and thermal Energies= -375.596199
Sum of electronic and thermal Enthalpies= -375.595255
Sum of electronic and thermal Free Energies= -375.638314

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	141.284	36.325	90.624

C,0,2.3331379286,0.7266960403,1.5883614546
C,0,2.7892296576,-0.2559261948,2.665000956
C,0,1.762700833,-0.9100858866,3.5965988894
C,0,0.4555366113,-0.104610152,3.7652717354
C,0,-0.0350059625,0.5481252942,2.4646893425
C,0,1.0382710648,1.4934003927,1.9059740943
B,0,2.84572067,-0.8097593636,4.8106989638
H,0,0.596664028,0.6877432953,4.514073392
H,0,3.4379227607,-1.0089994301,2.2109361613
H,0,2.1489217303,0.1058489655,0.7000576271
H,0,-0.3182380778,-0.7643237015,4.1772904159
H,0,-0.2671476434,-0.2248625478,1.7163743483
H,0,-0.9656643749,1.10224562,2.6418253248
H,0,1.2285947621,2.2917954231,2.6361830186
H,0,0.6866822533,1.9894286158,0.9926764653
H,0,3.1520693378,1.402218678,1.3084782746
O,0,3.7024576418,0.2862883721,3.7453157639
H,0,2.5642944638,-0.1702048504,5.793689757
H,0,3.6143392245,-1.7213121959,4.9671983581
H,0,1.5296769879,-1.9237868008,3.2487705264
C,0,3.719906808,1.6766890669,4.077878767
H,0,4.4191312162,1.7737910808,4.9108796709
H,0,4.0844064155,2.258926311,3.226712209
H,0,2.7347916636,2.0364319679,4.3902964838

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.207478	E(Thermal)=	0.216851
E(QCISD(T))=	-374.625135	E(Empiric)=	-0.175760
DE(Plus)=	-0.020530	DE(2DF)=	-0.351185
E(Delta-G3)=	-0.509352	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.474483	G3 Energy=	-375.465110
G3 Enthalpy=	-375.464166	G3 Free Energy=	-375.507832

6f-22 Product
B3LYP/6-31G**
E(RB3LYP) = -375.853095829

Zero-point correction= 0.211882 (Hartree/Particle)
Thermal correction to Energy= 0.221936
Thermal correction to Enthalpy= 0.222880
Thermal correction to Gibbs Free Energy= 0.177188
Sum of electronic and ZPE= -375.641214
Sum of electronic and thermal Energies= -375.631160
Sum of electronic and thermal Enthalpies= -375.630216
Sum of electronic and thermal Free Energies= -375.675908

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.267	38.301	96.167

C,0,2.0851329697,0.4453026847,1.0823121013
C,0,2.9665358806,-0.0704790285,2.2225470217
C,0,2.0874826815,-0.6725321054,3.3462038501
C,0,1.1264554853,0.415789968,3.8838777863
C,0,0.2299092127,0.9517866541,2.7558004062
C,0,1.0665305364,1.4839232792,1.5815393444
H,0,2.7521539593,-0.9719606624,4.1875499705
H,0,1.7021514026,1.2511031771,4.3098673323
O,0,3.8972505961,-0.9926417354,1.659539572
H,0,1.5652542001,-0.4139292707,0.6352703163
H,0,0.5147826922,0.0062957744,4.6957178353
H,0,-0.4233407109,0.1403703627,2.4006364795
H,0,-0.4314564421,1.7399869206,3.136130107
H,0,1.6038089404,2.3870764661,1.9058227602
H,0,0.4141844933,1.7925834637,0.7559189927
H,0,2.722823877,0.870880322,0.2993596605
H,0,3.5342506804,0.7826829308,2.6385926863
B,0,1.4237783778,-2.0608046286,3.0597759019
H,0,0.5071025776,-2.417760298,3.7452646753
H,0,1.8524541314,-2.8152458483,2.2405765407
C,0,5.0366224461,-1.2550579151,2.457467548
H,0,5.701549963,-1.8854377113,1.8623208023
H,0,5.5651764151,-0.3249468371,2.7190049577
H,0,4.7887526344,-1.7896429628,3.3860193516

B3LYP/6-31G*
E(RB3LYP) = -375.822215517
Zero-point correction= 0.213427 (Hartree/Particle)
Thermal correction to Energy= 0.223403
Thermal correction to Enthalpy= 0.224348
Thermal correction to Gibbs Free Energy= 0.178849
Sum of electronic and ZPE= -375.608788
Sum of electronic and thermal Energies= -375.598812
Sum of electronic and thermal Enthalpies= -375.597868
Sum of electronic and thermal Free Energies= -375.643366

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.188	37.956	95.760

C,0,2.0866038617,0.4451179329,1.0852485638
C,0,2.9685545952,-0.0706053416,2.2255990023
C,0,2.0898180716,-0.6689749096,3.3507672861
C,0,1.1239398604,0.4160573839,3.8844100602
C,0,0.2299563543,0.9494204463,2.7538181508
C,0,1.0691466135,1.484134049,1.5832088068
H,0,2.7554733244,-0.9620536224,4.193530183
H,0,1.6961875168,1.2531388458,4.3124844303
O,0,3.8883378564,-0.9980897911,1.6619056978
H,0,1.5651588901,-0.4143368387,0.6393688148
H,0,0.5099584222,0.0056000631,4.6946573903
H,0,-0.4193939108,0.1356035554,2.3956273533
H,0,-0.4358513312,1.735411078,3.1322285008
H,0,1.6072555049,2.3857210463,1.911573191
H,0,0.4186709803,1.796578736,0.7568567884
H,0,2.7248294984,0.8678487694,0.300555555
H,0,3.5385485093,0.7829816304,2.6388422865
B,0,1.4296621537,-2.0585865162,3.0579012435
H,0,0.5171394723,-2.42686697,3.7445977727
H,0,1.8556943946,-2.8068999582,2.229732919
C,0,5.028074252,-1.254885789,2.4540035734
H,0,5.6870539168,-1.8973999308,1.8635165918
H,0,5.5666733329,-0.3259633196,2.7030518356
H,0,4.7878548603,-1.7756075493,3.3936300028

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.204890	E(Thermal)=	0.215203
E(QCISD(T))=	-374.622923	E(Empiric)=	-0.175760
DE(Plus)=	-0.021435	DE(2DF)=	-0.350486

E(Delta-G3)=	-0.510824	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.476538	G3 Energy=	-375.466225
G3 Enthalpy=	-375.465280	G3 Free Energy=	-375.511414

6f-23 Product
B3LYP/6-31+G**
E(RB3LYP) = -375.854637102

Zero-point correction= 0.212086 (Hartree/Particle)
Thermal correction to Energy= 0.222025
Thermal correction to Enthalpy= 0.222969
Thermal correction to Gibbs Free Energy= 0.177544
Sum of electronic and ZPE= -375.642551
Sum of electronic and thermal Energies= -375.632612
Sum of electronic and thermal Enthalpies= -375.631668
Sum of electronic and thermal Free Energies= -375.677093

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.323	38.132	95.605

C,0,1.7596972018,0.5949516608,0.9725672604
C,0,2.8460502392,0.1852369711,1.9858673454
C,0,2.2086515546,-0.4957049667,3.2065678131
C,0,1.1404555081,0.4053130166,3.8673590065
C,0,0.0567192107,0.7954087876,2.8491133411
C,0,0.6699566804,1.4701986123,1.6117427565
H,0,3.0330279768,-0.651153385,3.942927821
H,0,1.6126934521,1.315458096,4.2567855573
H,0,3.5507461787,-0.5109218219,1.5028482017
H,0,1.312357249,-0.3278076326,0.574492151
H,0,0.6900936146,-0.1172998276,4.7192702288
H,0,-0.4907985628,-0.108239255,2.5383487369
H,0,-0.6801238862,1.4608710569,3.3155471081
H,0,1.1107920207,2.4304405557,1.9088837374
H,0,-0.1086893111,1.6939991786,0.8722164413
H,0,2.2101393425,1.1069254087,0.114026839
O,0,3.5922326858,1.3155595136,2.4653863432
B,0,1.8419583816,-1.9986113645,3.0265287108
H,0,1.0726968407,-2.5257652692,3.7775631117
H,0,2.394823121,-2.6770817382,2.2078278658
C,0,4.5128640488,1.8598203284,1.538121508

H,0,5.0890846632,2.6192250481,2.0723913603
H,0,5.2030032997,1.0892357359,1.1598674147
H,0,4.0166374898,2.3361772904,0.6806623399

B3LYP/6-31G*
E(RB3LYP) = -375.823618216

Zero-point correction= 0.213632 (Hartree/Particle)
Thermal correction to Energy= 0.223507
Thermal correction to Enthalpy= 0.224451
Thermal correction to Gibbs Free Energy= 0.179176
Sum of electronic and ZPE= -375.609986
Sum of electronic and thermal Energies= -375.600111
Sum of electronic and thermal Enthalpies= -375.599167
Sum of electronic and thermal Free Energies= -375.644443

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.253	37.795	95.290

C,0,1.7602531362,0.5820702172,0.9711350091
C,0,2.8494160807,0.1843878602,1.9858092616
C,0,2.2147882548,-0.4985822196,3.2080866034
C,0,1.1506893151,0.4071494191,3.8683338264
C,0,0.0660474887,0.798009567,2.8522090777
C,0,0.6779343746,1.4649938039,1.6106725259
H,0,3.0404840097,-0.65068584,3.9423519367
H,0,1.6284695398,1.3166691814,4.2529917783
H,0,3.5611452144,-0.5071471564,1.5052226135
H,0,1.3093432616,-0.3430361942,0.5814353392
H,0,0.7001369814,-0.110095619,4.7240428697
H,0,-0.4859985247,-0.1050976992,2.5464487153
H,0,-0.6676536823,1.4678889536,3.3184868361
H,0,1.1291365318,2.4219220878,1.9036072413
H,0,-0.1025976217,1.6936497668,0.8740238289
H,0,2.2077381221,1.0888264239,0.1071700054
O,0,3.5756241099,1.3220271942,2.4664647436
B,0,1.8300932097,-1.9974696231,3.0160673958
H,0,1.0513756187,-2.5231079196,3.7602054532
H,0,2.3757886777,-2.6770336775,2.1919459762
C,0,4.4979794619,1.8649711915,1.5462375248
H,0,5.0574604412,2.6404712547,2.0771178572
H,0,5.2061450041,1.1015868564,1.1842390491
H,0,4.0112699944,2.3238681708,0.6726075315

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205087	E(Thermal)=	0.215300
E(QCISD(T))=	-374.624600	E(Empiric)=	-0.175760
DE(Plus)=	-0.021381	DE(2DF)=	-0.350342
E(Delta-G3)=	-0.510938	(G3-Empiric)=	-0.175760
G3(0 K)=	-375.477935	G3 Energy=	-375.467722
G3 Enthalpy=	-375.466778	G3 Free Energy=	-375.512686

6f-24 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.856332456

Zero-point correction= 0.212420 (Hartree/Particle)
Thermal correction to Energy= 0.222572
Thermal correction to Enthalpy= 0.223516
Thermal correction to Gibbs Free Energy= 0.177555
Sum of electronic and ZPE= -375.643913
Sum of electronic and thermal Energies= -375.633760
Sum of electronic and thermal Enthalpies= -375.632816
Sum of electronic and thermal Free Energies= -375.678777

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.666	38.289	96.733

C,0,1.5637550854,0.3275276195,0.9745460309
C,0,2.6609177294,-0.2000257191,1.9086959863
C,0,2.0997882826,-0.6377753086,3.2659276606
C,0,1.3239234105,0.5360805196,3.9355409583
C,0,0.2269939147,1.0832348352,3.0042559513
C,0,0.7936919782,1.4849952154,1.6346764681
B,0,3.2184622906,-1.1260135264,4.2507667105
H,0,2.0205087452,1.3498722577,4.1847162114
O,0,3.3400652688,-1.3480328295,1.381504518
H,0,0.8778771329,-0.5002129133,0.7477513925
H,0,0.880131096,0.2035178286,4.8816140068
H,0,-0.5428364079,0.3110773786,2.8669690235
H,0,-0.2667582482,1.9419841293,3.4762929225
H,0,1.4675683251,2.3450513893,1.7603950305
H,0,-0.0141475136,1.8201969461,0.9731921115
H,0,1.9910056641,0.6614569151,0.0216273853

H,0,3.4071228892,0.5987451343,2.0736625604
H,0,2.9888489597,-1.9464718225,5.0922302137
H,0,4.3017349522,-0.6139036626,4.2371959615
H,0,1.3716151446,-1.4425732823,3.0825054558
C,0,4.237535104,-1.084887662,0.316215745
H,0,4.7647035077,-2.019334937,0.1095970522
H,0,3.7190854651,-0.765331353,-0.5983292831
H,0,4.9722182237,-0.3140321523,0.5951549265

B3LYP/6-31G*
E(RB3LYP) = -375.825441275

Zero-point correction= 0.213962 (Hartree/Particle)
Thermal correction to Energy= 0.224126
Thermal correction to Enthalpy= 0.225070
Thermal correction to Gibbs Free Energy= 0.178670
Sum of electronic and ZPE= -375.611479
Sum of electronic and thermal Energies= -375.601315
Sum of electronic and thermal Enthalpies= -375.600371
Sum of electronic and thermal Free Energies= -375.646772

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.641	37.944	97.658

C,0,1.55305787,0.3162987356,0.9770828695
C,0,2.6471513753,-0.1943975875,1.9220361786
C,0,2.0759831424,-0.6252964746,3.2792411687
C,0,1.321788353,0.5629309545,3.9376824459
C,0,0.2251375052,1.1044820075,3.0038749919
C,0,0.7865803948,1.483301109,1.6250981354
B,0,3.2415924047,-1.1559881888,4.1907139823
H,0,2.0321694088,1.3694572813,4.1709489848
O,0,3.3401399026,-1.3458549324,1.4265627253
H,0,0.8673215089,-0.5142180065,0.7599572851
H,0,0.8799564683,0.2510633148,4.8924417955
H,0,-0.5514855935,0.3361250948,2.8811420405
H,0,-0.2621185203,1.9737285503,3.4643299202
H,0,1.4641964572,2.3428925286,1.7355936375
H,0,-0.0235369368,1.8122872956,0.962603043
H,0,1.9811277247,0.6385140326,0.0196051475
H,0,3.3827528605,0.6141683274,2.0861421059
H,0,3.1328116845,-2.1429485374,4.8605421519
H,0,4.2566230739,-0.5220069454,4.2779692408

H,0,1.337647283,-1.4183228509,3.0875786183
C,0,4.2406729725,-1.0928107685,0.3658813469
H,0,4.7769222639,-2.0266473204,0.1763000599
H,0,3.7278904933,-0.7907873881,-0.5587333925
H,0,4.9694289033,-0.3108252315,0.6321105171

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205404	E(Thermal)=	0.215897
E(QCISD(T))=	-374.626140	E(Empiric)=	-0.175760
DE(Plus)=	-0.021807	DE(2DF)=	-0.349886
E(Delta-G3)=	-0.510164	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.478353	G3 Energy=	-375.467860
G3 Enthalpy=	-375.466916	G3 Free Energy=	-375.513952

6f-25 Product
E(RB3LYP) = -375.829981868

Zero-point correction= 0.215900 (Hartree/Particle)
Thermal correction to Energy= 0.225024
Thermal correction to Enthalpy= 0.225969
Thermal correction to Gibbs Free Energy= 0.182541
Sum of electronic and zero-point Energies= -375.614082
Sum of electronic and thermal Energies= -375.604957
Sum of electronic and thermal Enthalpies= -375.604013
Sum of electronic and thermal Free Energies= -375.647440

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	141.205	36.277	91.400

C,0,2.321564829,0.6268070105,1.3526771179
C,0,2.866524803,-0.2457287445,2.4766147357
C,0,1.931874411,-0.7758005534,3.5718897574
C,0,0.6996885106,0.1209705672,3.8232528965
C,0,0.0963177501,0.7192013858,2.5437047954
C,0,1.1580133162,1.5293086631,1.7866721857
B,0,3.1543436604,-0.6060196966,4.6331846776
H,0,0.9794194983,0.9514201714,4.4856335823
H,0,3.4908883011,-1.0523693527,2.0721177075
H,0,1.9676719177,-0.0629942012,0.5726226083
H,0,-0.0558399819,-0.4568667843,4.370249814
H,0,-0.2876369714,-0.0802018116,1.8913853709
H,0,-0.7597745459,1.359649016,2.7918729702

H,0,1.5334189456,2.3307364772,2.4378178885
H,0,0.7271142706,2.0158962489,0.9027975449
H,0,3.1338844326,1.2098768857,0.8964489314
O,0,3.7409123604,0.5110501644,3.4256192614
H,0,3.0091513533,0.0119870071,5.6547912104
H,0,3.9874123604,-1.4813711091,4.6451973072
H,0,1.6205246077,-1.8023287848,3.3486859418
C,0,5.124974284,0.6425169268,3.1012012687
H,0,5.6009557639,1.1423175747,3.9470613309
H,0,5.5797650784,-0.3437614921,2.9500182495
H,0,5.2355560451,1.2545764315,2.200442846

B3LYP/6-31G*
E(RB3LYP) = -375.855814792 A.U. after 1 cycles

Zero-point correction= 0.212395 (Hartree/Particle)
Thermal correction to Energy= 0.222481
Thermal correction to Enthalpy= 0.223425
Thermal correction to Gibbs Free Energy= 0.176124
Sum of electronic and zero-point Energies= -375.643420
Sum of electronic and thermal Energies= -375.633334
Sum of electronic and thermal Enthalpies= -375.632390
Sum of electronic and thermal Free Energies= -375.679691

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	139.609	38.036	99.554

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.207265	E(Thermal)=	0.216729
E(QCISD(T))=	-374.634241	E(Empiric)=	-0.175760
DE(Plus)=	-0.020517	DE(2DF)=	-0.350487
E(Delta-G3)=	-0.509067	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.482807	G3 Energy=	-375.473343
G3 Enthalpy=	-375.472398	G3 Free Energy=	-375.516430

6f-26 Product
B3LYP/6-31+G**
E(RB3LYP) = -375.853377750

Zero-point correction= 0.211883 (Hartree/Particle)
Thermal correction to Energy= 0.222016
Thermal correction to Enthalpy= 0.222961

Thermal correction to Gibbs Free Energy= 0.176988
Sum of electronic and ZPE= -375.641495
Sum of electronic and thermal Energies= -375.631361
Sum of electronic and thermal Enthalpies= -375.630417
Sum of electronic and thermal Free Energies= -375.676390

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	139.317	38.316	96.758

C,0,1.7156543919,0.4408240523,0.9182008161
C,0,2.8181602437,-0.0578118231,1.8670647304
C,0,2.1991515338,-0.6426655581,3.1472744135
C,0,1.3490525113,0.4375263885,3.8605817721
C,0,0.2400751421,0.9604346532,2.9319519718
C,0,0.8203540276,1.4849605248,1.6090212445
H,0,3.0386972379,-0.9150597353,3.8222944844
H,0,1.989261634,1.2804898019,4.1600966294
O,0,3.6479151882,-1.0600847658,1.2788628608
H,0,1.1170835455,-0.4263130815,0.6054915248
H,0,0.9161340451,0.0264846946,4.7795243275
H,0,-0.469653796,0.1458712487,2.7217159341
H,0,-0.3333821226,1.7510650351,3.4314009712
H,0,1.4129412935,2.3888859789,1.8128778979
H,0,0.0136262428,1.7912970326,0.9322114967
H,0,2.1524969013,0.8704050737,0.0091227133
H,0,3.4579456641,0.8022160917,2.140735045
B,0,1.5003722838,-2.0396806535,3.0219383508
H,0,0.8730808367,-2.4425830294,3.9616016642
H,0,1.6094265575,-2.7429888433,2.0649723385
C,0,4.5944827798,-0.5796530627,0.3416104203
H,0,5.2171605013,-1.4312928109,0.0572484776
H,0,4.1214998406,-0.1743146528,-0.5639149406
H,0,5.235537516,0.1998504403,0.7828028554

B3LYP/6-31G*
E(RB3LYP) = -375.822283504

Zero-point correction= 0.213386 (Hartree/Particle)
Thermal correction to Energy= 0.223461
Thermal correction to Enthalpy= 0.224405
Thermal correction to Gibbs Free Energy= 0.178561
Sum of electronic and ZPE= -375.608897
Sum of electronic and thermal Energies= -375.598822

Sum of electronic and thermal Enthalpies= -375.597878
Sum of electronic and thermal Free Energies= -375.643723

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	140.224	37.994	96.488

C,0,1.7208784615,0.4438204069,0.9212892139
C,0,2.8236286605,-0.0534994094,1.8707510656
C,0,2.2028547514,-0.6382115823,3.1507079984
C,0,1.3470991942,0.4376007584,3.8619088912
C,0,0.2401223851,0.9574686841,2.9302593495
C,0,0.8237105437,1.4858839884,1.6108666653
H,0,3.0424393011,-0.9069394436,3.8270071809
H,0,1.9836162379,1.2824974393,4.1650468048
O,0,3.6480347234,-1.0584130985,1.289914445
H,0,1.1234474366,-0.4242336708,0.6076694023
H,0,0.9115119061,0.0244426132,4.7792443155
H,0,-0.4655065983,0.1397951959,2.7156854074
H,0,-0.3391049457,1.744955981,3.4289752561
H,0,1.4160806724,2.3893248638,1.8193622757
H,0,0.0185241944,1.7949129347,0.9326694194
H,0,2.1578897701,0.8732387514,0.0114262337
H,0,3.4610474083,0.8093550598,2.1435456153
B,0,1.50549849,-2.0360421375,3.016017309
H,0,0.87154509,-2.4462551172,3.9491914899
H,0,1.6199749194,-2.7374639793,2.0566068746
C,0,4.5827721392,-0.586449591,0.343207079
H,0,5.2103946257,-1.4381795866,0.0663788013
H,0,4.1065719657,-0.1948354936,-0.5679803333
H,0,5.2240426672,0.2050894328,0.7649372394

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.204851	E(Thermal)=	0.215260
E(QCISD(T))=	-374.622912	E(Empiric)=	-0.175760
DE(Plus)=	-0.021590	DE(2DF)=	-0.350277
E(Delta-G3)=	-0.510963	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.476651	G3 Energy=	-375.466242
G3 Enthalpy=	-375.465298	7G3 Free Energy=	-375.511779

6f-27 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.821288842

Zero-point correction= 0.206196 (Hartree/Particle)
Thermal correction to Energy= 0.218131
Thermal correction to Enthalpy= 0.219075
Thermal correction to Gibbs Free Energy= 0.165658
Sum of electronic and zero-point Energies= -375.615093
Sum of electronic and thermal Energies= -375.603158
Sum of electronic and thermal Enthalpies= -375.602213
Sum of electronic and thermal Free Energies= -375.655631

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	136.879	40.777	112.426

C,0,-2.28867,0.81509,0.40806
C,0,-1.7763,0.80129,-1.03684
C,0,-0.93992,-0.45799,-1.3031
C,0,0.03234,-0.73848,-0.18462
C,0,-0.02932,-0.15526,1.02435
C,0,-1.11559,0.82814,1.40008
O,0,0.95435,-1.67021,-0.58069
C,0,1.91152,-2.09895,0.37211
H,0,1.42774,-2.54081,1.25366
B,0,3.00875,2.68323,-0.17722
H,0,-0.69684,1.84559,1.46229
H,0,-1.59413,-1.33317,-1.43146
H,0,-1.48189,0.60117,2.41109
H,0,-2.90114,-0.08114,0.5801
H,0,-2.93827,1.68181,0.5808
H,0,-1.15803,1.69319,-1.20949
H,0,-2.60951,0.85199,-1.74801
H,0,-0.37624,-0.36529,-2.24003
H,0,3.46142,2.10721,-1.11959
H,0,2.13912,3.48686,-0.32956
H,0,3.43517,2.46663,0.91687
H,0,0.70604,-0.38984,1.78837
H,0,2.52219,-2.85379,-0.12746
H,0,2.55314,-1.26893,0.69836

B3LYP/6-31+G*
E(RB3LYP) = -375.789125872

Zero-point correction= 0.207360 (Hartree/Particle)
Thermal correction to Energy= 0.218581
Thermal correction to Enthalpy= 0.219525
Thermal correction to Gibbs Free Energy= 0.167684
Sum of electronic and ZPE= -375.581765
Sum of electronic and thermal Energies= -375.570545
Sum of electronic and thermal Enthalpies= -375.569601
Sum of electronic and thermal Free Energies= -375.621442

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.162	38.642	109.109

C,0,-2.28867,0.81509,0.40806
C,0,-1.7763,0.80129,-1.03684
C,0,-0.93992,-0.45799,-1.3031
C,0,0.03234,-0.73848,-0.18462
C,0,-0.02932,-0.15526,1.02435
C,0,-1.11559,0.82814,1.40008
O,0,0.95435,-1.67021,-0.58069
C,0,1.91152,-2.09895,0.37211
H,0,1.42774,-2.54081,1.25366
B,0,3.00875,2.68323,-0.17722
H,0,-0.69684,1.84559,1.46229
H,0,-1.59413,-1.33317,-1.43146
H,0,-1.48189,0.60117,2.41109
H,0,-2.90114,-0.08114,0.5801
H,0,-2.93827,1.68181,0.5808
H,0,-1.15803,1.69319,-1.20949
H,0,-2.60951,0.85199,-1.74801
H,0,-0.37624,-0.36529,-2.24003
H,0,3.46142,2.10721,-1.11959
H,0,2.13912,3.48686,-0.32956
H,0,3.43517,2.46663,0.91687
H,0,0.70604,-0.38984,1.78837
H,0,2.52219,-2.85379,-0.12746
H,0,2.55314,-1.26893,0.69836

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199066	E(Thermal)=	0.210585
E(QCISD(T))=	-374.584045	E(Empiric)=	-0.175760

DE(Plus)=	-0.022773	DE(2DF)=	-0.347390
E(Delta-G3)=	-0.511692	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.442594	G3 Energy=	-375.431075
G3 Enthalpy=	-375.430130	G3 Free Energy=	-375.482619

6f-28 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.81642208

Zero-point correction= 0.206723 (Hartree/Particle)
Thermal correction to Energy= 0.218120
Thermal correction to Enthalpy= 0.219064
Thermal correction to Gibbs Free Energy= 0.169248
Sum of electronic and zero-point Energies= -375.609700
Sum of electronic and thermal Energies= -375.598302
Sum of electronic and thermal Enthalpies= -375.597358
Sum of electronic and thermal Free Energies= -375.647174

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	136.872	40.507	104.847

B3LYP/6-31+G*
E(RB3LYP) = -375.785525323

Zero-point correction= 0.208044 (Hartree/Particle)
Thermal correction to Energy= 0.219517
Thermal correction to Enthalpy= 0.220461
Thermal correction to Gibbs Free Energy= 0.170200
Sum of electronic and ZPE= -375.577482
Sum of electronic and thermal Energies= -375.566009
Sum of electronic and thermal Enthalpies= -375.565064
Sum of electronic and thermal Free Energies= -375.615325

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	137.749	40.354	105.783

C,0,0.29702,0.39627,-1.19273
C,0,1.69308,0.95088,-1.07174
C,0,2.47923,0.29676,0.07492
C,0,1.61082,0.17262,1.33268

C,0,0.3753,-0.70463,1.06908
C,0,-0.29032,-0.33128,-0.2354
O,0,-1.62228,-0.67772,-0.40377
C,0,-1.97332,-2.02428,-0.10465
B,0,-2.39314,2.13363,0.2114
H,0,-1.80965,-2.27258,0.95169
H,0,1.64193,2.04056,-0.91575
H,0,0.66672,-1.76604,1.06019
H,0,2.23007,0.81576,-2.02071
H,0,2.80862,-0.70495,-0.23502
H,0,3.38585,0.87531,0.28976
H,0,1.27853,1.1724,1.64314
H,0,2.19055,-0.24286,2.16573
H,0,-0.34971,-0.59237,1.88605
H,0,-3.50895,1.77556,-0.01247
H,0,-1.9216,1.97231,1.29701
H,0,-1.7806,2.73488,-0.6176
H,0,-0.27799,0.62996,-2.08597
H,0,-3.03799,-2.11916,-0.32861
H,0,-1.40841,-2.72886,-0.73086

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199722	E(Thermal)=	0.211516
E(QCISD(T))=	-374.582968	E(Empiric)=	-0.175760
DE(Plus)=	-0.022875	DE(2DF)=	-0.347887
E(Delta-G3)=	-0.510309	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.440076	G3 Energy=	-375.428282
G3 Enthalpy=	-375.427338	G3 Free Energy=	-375.478279

6f-29 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.826197251

Zero-point correction=	0.207616 (Hartree/Particle)
Thermal correction to Energy=	0.218535
Thermal correction to Enthalpy=	0.219479
Thermal correction to Gibbs Free Energy=	0.171273
Sum of electronic and zero-point Energies=	-375.618582
Sum of electronic and thermal Energies=	-375.607662
Sum of electronic and thermal Enthalpies=	-375.606718
Sum of electronic and thermal Free Energies=	-375.654925

C,0,1.16092,0.89272,1.24645
C,0,2.12957,0.88589,0.05563
C,0,2.17061,-0.49723,-0.60484
C,0,0.78269,-0.89514,-1.12724
C,0,-0.30918,-0.61097,-0.12383
C,0,-0.16409,0.23359,0.92314
O,0,-1.42519,-1.32867,-0.42375
C,0,-2.55475,-1.20363,0.42941
B,0,-1.5523,2.44288,-0.43047
H,0,-2.9242,-0.17129,0.44806
H,0,1.62456,0.36987,2.09911
H,0,0.55304,-0.3554,-2.05719
H,0,0.99191,1.92206,1.58534
H,0,1.80117,1.63041,-0.6824
H,0,3.13179,1.18466,0.38615
H,0,2.50894,-1.23984,0.13117
H,0,2.89493,-0.5162,-1.42781
H,0,0.74613,-1.9618,-1.37903
H,0,-1.42355,2.07823,-1.5604
H,0,-2.57949,2.23672,0.14573
H,0,-0.72304,3.13864,0.07407
H,0,-0.96288,0.34918,1.64975
H,0,-3.32018,-1.86119,0.01352
H,0,-2.31399,-1.5204,1.45258

B3LYP/6-31+G*
E(RB3LYP) = -375.795527805

Zero-point correction= 0.208852 (Hartree/Particle)
Thermal correction to Energy= 0.218974
Thermal correction to Enthalpy= 0.219918
Thermal correction to Gibbs Free Energy= 0.173623
Sum of electronic and ZPE= -375.586676
Sum of electronic and thermal Energies= -375.576554
Sum of electronic and thermal Enthalpies= -375.575609
Sum of electronic and thermal Free Energies= -375.621905

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.408	37.764	97.436

C,0,1.16092,0.89272,1.24645
C,0,2.12957,0.88589,0.05563
C,0,2.17061,-0.49723,-0.60484

C,0,0.78269,-0.89514,-1.12724
C,0,-0.30918,-0.61097,-0.12383
C,0,-0.16409,0.23359,0.92314
O,0,-1.42519,-1.32867,-0.42375
C,0,-2.55475,-1.20363,0.42941
B,0,-1.5523,2.44288,-0.43047
H,0,-2.9242,-0.17129,0.44806
H,0,1.62456,0.36987,2.09911
H,0,0.55304,-0.3554,-2.05719
H,0,0.99191,1.92206,1.58534
H,0,1.80117,1.63041,-0.6824
H,0,3.13179,1.18466,0.38615
H,0,2.50894,-1.23984,0.13117
H,0,2.89493,-0.5162,-1.42781
H,0,0.74613,-1.9618,-1.37903
H,0,-1.42355,2.07823,-1.5604
H,0,-2.57949,2.23672,0.14573
H,0,-0.72304,3.13864,0.07407
H,0,-0.96288,0.34918,1.64975
H,0,-3.32018,-1.86119,0.01352
H,0,-2.31399,-1.5204,1.45258

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.200498	E(Thermal)=	0.210947
E(QCISD(T))=	-374.591069	E(Empiric)=	-0.175760
DE(Plus)=	-0.022108	DE(2DF)=	-0.348613
E(Delta-G3)=	-0.511588	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.448640	G3 Energy=	-375.438192
G3 Enthalpy=	-375.437247	G3 Free Energy=	-375.484173

6f-30 Variational Transition State
B3LYP/6-31+G**
E(RB3LYP) = -375.817541236

Zero-point correction=	0.206695 (Hartree/Particle)
Thermal correction to Energy=	0.218041
Thermal correction to Enthalpy=	0.218985
Thermal correction to Gibbs Free Energy=	0.169583
Sum of electronic and zero-point Energies=	-375.610846
Sum of electronic and thermal Energies=	-375.599500
Sum of electronic and thermal Enthalpies=	-375.598556
Sum of electronic and thermal Free Energies=	-375.647959

C,0,-0.14822,-0.52248,0.37021
C,0,0.12575,0.58485,1.08252
C,0,1.32178,1.46565,0.8143
C,0,1.94366,1.20033,-0.56505
C,0,2.06482,-0.30565,-0.8266
C,0,0.6853,-0.98584,-0.80536
O,0,-1.16922,-1.33868,0.79885
C,0,-2.02403,-1.88999,-0.19643
B,0,-2.52843,1.91938,-0.2815
H,0,-1.48549,-2.54339,-0.89461
H,0,2.07741,1.30131,1.59991
H,0,0.15595,-0.78668,-1.74884
H,0,1.03354,2.52159,0.90031
H,0,1.31085,1.65162,-1.34173
H,0,2.92598,1.68285,-0.63569
H,0,2.6995,-0.75675,-0.05159
H,0,2.55626,-0.49627,-1.78822
H,0,0.80408,-2.0759,-0.74612
H,0,-3.23667,1.361,0.50035
H,0,-1.98687,2.93927,0.02168
H,0,-2.42475,1.50259,-1.39706
H,0,-0.49676,0.80229,1.9496
H,0,-2.76617,-2.48475,0.34047
H,0,-2.53569,-1.10037,-0.76203

B3LYP/6-31+G*
E(RB3LYP) = -375.786648638

Zero-point correction= 0.207974 (Hartree/Particle)
Thermal correction to Energy= 0.219414
Thermal correction to Enthalpy= 0.220358
Thermal correction to Gibbs Free Energy= 0.170480
Sum of electronic and ZPE= -375.578674
Sum of electronic and thermal Energies= -375.567235
Sum of electronic and thermal Enthalpies= -375.566291
Sum of electronic and thermal Free Energies= -375.616169

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.684	40.387	104.978

C,0,-0.14822,-0.52248,0.37021
C,0,0.12575,0.58485,1.08252

C,0,1.32178,1.46565,0.8143
C,0,1.94366,1.20033,-0.56505
C,0,2.06482,-0.30565,-0.8266
C,0,0.6853,-0.98584,-0.80536
O,0,-1.16922,-1.33868,0.79885
C,0,-2.02403,-1.88999,-0.19643
B,0,-2.52843,1.91938,-0.2815
H,0,-1.48549,-2.54339,-0.89461
H,0,2.07741,1.30131,1.59991
H,0,0.15595,-0.78668,-1.74884
H,0,1.03354,2.52159,0.90031
H,0,1.31085,1.65162,-1.34173
H,0,2.92598,1.68285,-0.63569
H,0,2.6995,-0.75675,-0.05159
H,0,2.55626,-0.49627,-1.78822
H,0,0.80408,-2.0759,-0.74612
H,0,-3.23667,1.361,0.50035
H,0,-1.98687,2.93927,0.02168
H,0,-2.42475,1.50259,-1.39706
H,0,-0.49676,0.80229,1.9496
H,0,-2.76617,-2.48475,0.34047
H,0,-2.53569,-1.10037,-0.76203

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.199655	E(Thermal)=	0.211418
E(QCISD(T))=	-374.582749	E(Empiric)=	-0.175760
DE(Plus)=	-0.022797	DE(2DF)=	-0.347956
E(Delta-G3)=	-0.510696	E(G3-Empiric)=	-0.175760
G3(0 K)=	-375.440303	G3 Energy=	-375.428540
G3 Enthalpy=	-375.427595	G3 Free Energy=	-375.478155

A. 6. Listing of Dynamics Programs for Program Suite PROGDYN

1. Program progdynstarterHP

```
#!/bin/bash
# This is the master control program for dynamics, in the form of a Unix Shell Script.
#
# Necessary input files:
# freqinHP          - This is the standard output from a Gaussian 98 or 03 frequency
calculation using freq=hpmodes.
# progdyn.conf – This is a file giving a variety of configuration options, called on by
many of the subprograms.
#
# Optional input:
# isomernumber      - A number in file isomernumber provides a start for numbering runs.
# detour – A signal file that, by existing, signals the program to do a side calculations
# nogo – A signal file that, by existing, signals the program to stop between points
#
# Programs called:
#  proggenHP      - An awk program that starts a trajectory, giving each mode its zero
point energy (if a quasiclassical calculation) plus random additional excitations
depending on the temperature.
#  prog1stpoint – Awk program that creates the first Gaussian input file for each run
#  prog2ndpoint – Awk program that creates the second Gaussian input file for each run
#  progdynb – Creates subsequent Gaussian input files until run is completed, used the
awk
# proganal – A program to analyze the latest point and see if a run is done.  This
program must be redone for each new system.  Elaborate changes are often programmed
into proganal, such as the automatic changing of configuration variables.
# randgen – A program that generates random numbers between 0 and 1.  These are
generated all at once and stored in a file for use by proggenHP.
#
# Output files
# isomernumber – A running tab of the run number
# geoRecord – A record of all the starting positions and velocities.
# geoPlusVel – Created by proggen, this gives starting position and velocities for current
run.
# g03.com – Created by prog1stpoint, prog2ndpoint, and progdynb, this is the latest
input
#       file for Gaussian03 for current run and latest point.
# olddynrun and olderdynrun – files containing the last two outputs from Gaussian, for
creation
# of the next point
# dyn  - A record of all of the Gaussian outputs.
```

```
# dynfollowfile – A short record of the runs and their results.
# skipstart - A signal file that, by existing, tells progdynstarterHP that we are in the middle of a run.
# diagnostics – optional output that follows which subprograms are running and configuration variables, decided by variable in progdyn.conf
# vellist – optional output that list the velocities of each atom, decided by variable in progdyn.conf
# A number of files starting with 'temp' are created then later erased.


#progdynstarterHP, made to use high=precision modes from Gaussian freq output
#updated to create a random number file temp811 that is used by proggenHP
#version September 16, 2005, made for workstations
#version August 2007 to allow periodic copying of g03.log to dyn putting it under control of progdynb
#version Feb 2008 moves variables like the scratch directory and location of randgen to the beginning
#version March 2008 added proganal reporting to points 1 and 2
#                                   OUTLINE
# A. initilize to perform Gaussian jobs and know where we are
#    start loop
# B. if no file named "skipstart" then generate a new isomer.  Get rid of skipstart to start new isomer.
#
#  AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
#origdir, randdir, scratchdir, g03root, logfile, randdir all may need varied from system to system and assigned here or by program calling this one
export g03root=/usr/local/g03
source $g03root/g03/bsd/g03.profile
origdir=`pwd`
cd $origdir
logfile=docslog
randdir=~/bin
scratchdir=$TMPDIR

rm -f nogo    # assume that if someone is starting a job, they want it to go.
rm -f diagnostics # contains extra info from start of progFS

while (true)
do
#  BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
if (test -f skipstart) then
  echo "skipping start and continuing from previous runs"
else
```

```
# change from older versions - freqin and most other files are in origdir.  Advantage is
compartmentalization.
# Also allows separate configurations for separate runs, so we can move to using config
files.
# Disadvantage is multiple copies of files.
  cd $origdir
  echo 3 > runpointnumber
  $randdir/randgen > temp811
# lets keep the next 8 lines as the only difference between progdynstarter and
progdynstarterHP
   awk '/       1       2       3       4/,/Harmonic frequencies/ {print}' freqinHP >
temp401
   awk '/Frequencies --/ {print $3;print $4;print $5;print $6;print $7}' temp401 >
tempfreqs
   awk '/Reduced masses/ {print $4;print $5;print $6;print $7;print $8}' temp401 >
tempredmass
   awk '/Force constants/ {print $4;print $5;print $6;print $7;print $8}' temp401 >
tempfrc
   awk '/0/ && ((length($1) < 2) && ($1 < 4)) {print}' temp401 > tempmodes
   awk '/has atomic number/ {print}' freqinHP > tempmasses
   awk '/Standard orientation:/,/tional const/ {if ($3==0) print}' freqinHP > tempstangeos
   awk -f proggenHP freqinHP > geoPlusVel
  if (test -f isomernumber) then
    cp isomernumber temp533
    awk 'BEGIN {getline;i=$1+1;print i}' temp533 > isomernumber
    rm temp533
  else
    echo 1 > isomernumber
  fi
  rm g03.com
  awk -f prog1stpoint geoPlusVel > g03.com
# TO DO - put error checking in prog1stpoint, prog2ndpoint, and progdynb  so no
g03.com unless things are ok
  if (test -s g03.com) then
    rm tempfreqs tempredmass tempfrc tempmodes tempstangeos tempmasses temp401
temp811
    cat isomernumber >> geoRecord
    cat geoPlusVel >> geoRecord
    cat g03.com
    rm -f goingwell
    cd $scratchdir
    $g03root/g03/g03 $origdir/g03.com > $origdir/g03.log
    cd $origdir
    grep 'Normal termination' g03.log > goingwell
```

```
    if (test -s goingwell) then
      cat g03.log >> dyn
      awk -f proganal g03.log >> dynfollowfile
      cp g03.log olderdynrun
    else
      break
    fi
  else
    break
  fi
  rm g03.com
  awk -f prog2ndpoint g03.log > g03.com
  if (test -s g03.com) then
    rm -f goingwell
    cd $scratchdir
    $g03root/g03/g03 $origdir/g03.com > $origdir/g03.log
    cd $origdir
    grep 'Normal termination' g03.log > goingwell
    if (test -s goingwell) then
      cp g03.log olddynrun
      cat g03.log >> dyn
      awk -f proganal g03.log >> dynfollowfile
# old program progdyn replaced here with commands from progdyn
      awk '/Input orientation/,/Distance matrix/ {print}' olddynrun > temp101
      awk '/   0   / {print}' temp101 > old
      awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun > temp102
      awk '/   0   / {print}' temp102 > older
      awk -f progdynb olddynrun > g03.com
      rm -f temp101 temp102 old older tempchk
    else
      break
    fi
  else
    break
  fi
# we've just completed a start, so lets skipstart until instructed otherwise
  echo "skipping start" > skipstart
fi

while (true)
do
#increment runpointnumber
  if (test -f runpointnumber) then
    cp runpointnumber temp533
```

```
    awk 'BEGIN {getline;i=$1+1;print i}' temp533 > runpointnumber
    rm temp533
  else
    echo 4 > runpointnumber
  fi
# this loop always starts with a g03.com in place - because of the loss of former program
progdyn, I
# may have to worry about how each it is to restart from a bad run
  rm -f goingwell
  cd $scratchdir
  $g03root/g03/g03 $origdir/g03.com > $origdir/g03.log
  cd $origdir
  grep 'Normal termination' g03.log > goingwell
  if (test -s goingwell) then
    cp olddynrun olderdynrun
    cp g03.log olddynrun
# old program progdyn replaced here too
    awk '/Input orientation/,/Distance matrix/ {print}' olddynrun > temp101
    awk '/   0   / {print}' temp101 > old
    awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun > temp102
    awk '/   0   / {print}' temp102 > older
    awk -f progdynb olddynrun > g03.com
    rm -f temp101 temp102 old older tempchk
# line removed to move the command under control of progdynb      cat g03.log >> dyn
  else
    break
  fi

# here is a cool link that lets you interupt the dynamics with a short job, then
# it automatically goes back to the dynamics  just make the file 'detour' and it
# will delete detour, run run.com, then go back to dynamics
  if (test  -f detour) then
    rm detour
    date >> $logfile
    cat run.com >> $logfile
    cp run.log temp.log
    cd $scratchdir
    $g03root/g03/g03 $origdir/run.com > $origdir/run.log
    cd $origdir
  fi

#stop it all nicely by creating a nogo file
  if (test  -f nogo) then
    break
```

```
  fi

#figure out if this isomer is done
  awk -f proganal g03.log >> dynfollowfile
  rm -f tempdone
  awk -f proganal g03.log > temp281
  awk '/XXXX/ {print}' temp281 > tempdone
  rm temp281
  if (test  -s tempdone) then
    rm -f skipstart
    rm -f olddynrun
    rm -f olderdynrun
    rm -f geoPlusVel
    break
  fi
done

# We've got to break a second time to get out of this loop
# if we really want to quit.  Otherwise, it will start over
# at the top
if (test  -f nogo) then
  break
fi
if (test  -s goingwell) then
  echo "probably starting a new point"
else
  break
fi
done
exit 0
```

2. Program proggenHP

```
BEGIN {
# updated June 2008 to incorportate new method for choosing displacements with
initialdis 2
# updated Jan 17 2008 - bug fix for > 99 atoms, 300 excitations of low modes possible
# version August 2007 - incorporates classical trajectory calculation option
#also allows listing of number of imaginary frequencies
# version Sept 16, 2005 - incorportates searchdir but not yet rotation
# now reads random numbers from temp811, starting at a random place
# The input files are generated before this and are tempfreqs, tempredmass,
# tempfrc, tempmodes, and tempstangeos.
# It will count the number of atoms.
```

```
# Gets from progdyn.conf
# timestep, scaling, temp, and initialdis.
# default values
initialDis=0
timeStep=1E-15
scaling=1.0
temp=298.15
#default is quassiclassical
classical=0
#default is starting from transition state
numimag=1

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="initialdis") initialDis=$2
  if ($1=="timestep") timeStep=$2
  if ($1=="scaling") scaling=$2
  if ($1=="temperature") temp=$2
  if ($1=="searchdir") searchdir=$2
  if ($1=="classical") classical=$2
  if ($1=="numimag") numimag=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag==1) print "***************** starting proggen ****************" >>
"diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
```

```
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title,initialdis,timestep,scaling,temperature" >>
"diagnostics"
if (diag==1) print
processors,checkpoint,title1,title2,title3,title4,initialDis,timeStep,scaling,temp >>
"diagnostics"

i=1;j=1;k=1
c=29980000000
h=6.626075E-34
avNum=6.02E23
numAtoms=0

# put geometries into array, also figure out number of atoms
# note that this picks out the last geometry in a file, assuming
# that if there is an optimization followed by a freq, nothing else follows
# kludgy - repeats last line twice - must be a better way
do {
  getline < "tempstangeos"
  if (oldline==$0) $0=""
  oldline=$0
  atom = $1
  if (atom>numAtoms) numAtoms=atom
  atNum[atom]=$2
  geoArr[atom,1]=$4
  geoArr[atom,2]=$5
  geoArr[atom,3]=$6
  velArr[atom,1]=0
  velArr[atom,2]=0
  velArr[atom,3]=0
  }
while (length($0) > 0)

#output the number of atoms - this will help in reading the file later
print numAtoms

# put in atomic symbols and atomic weights - this will have to be edited for isotopic
labeling
for (i=1;i<=numAtoms;i++) {
  getline < "tempmasses"
  if (i<100) atWeight[i]=$9
  if (i>99) atWeight[i]=$8
  if (atNum[i]==1) atSym[i]="H"
  if (atNum[i]==5) atSym[i]="B"
```

```
   if (atNum[i]==6) atSym[i]="C"
   if (atNum[i]==7) atSym[i]="N"
   if (atNum[i]==8) atSym[i]="O"
   if (atNum[i]==9) atSym[i]="F"
   if (atNum[i]==13) atSym[i]="Al"
   if (atNum[i]==17) atSym[i]="Cl"

#   print atNum[i],atSym[i],atWeight[i],geoArr[i,1],geoArr[i,2],geoArr[i,3]
   }

# read in frequencies, scale them, read in Reduced masses, read in force
#constants, replace negative frequencies by 8 wavenumbers
numFreq=3*numAtoms-6
for (i=1;i<=numFreq;i++) {
   getline < "tempfreqs"
   freq[i]=$0*scaling
   if (freq[i]<0) freq[i]=8
   }
for (i=1;i<=numFreq;i++) {
   getline < "tempredmass"
   redMass[i]=$0
   }
for (i=1;i<=numFreq;i++) {
   getline < "tempfrc"
   frc[i]=$0
   if (frc[i]==0) frc[i]=0.0001
#   print freq[i],redMass[i],frc[i]
   }

# read in the modes
#the next 10 lines are commented for low precision modes, uncommented for high
precision modes
for (i=1;i<=numFreq;i+=5) {
   for (j=1;j<=(3*numAtoms);j++) {
      getline < "tempmodes"
      mode[i,$2,$1]=$4
      mode[i+1,$2,$1]=$5
      mode[i+2,$2,$1]=$6
      mode[i+3,$2,$1]=$7
      mode[i+4,$2,$1]=$8
      }
   }
#the next 14 lines are uncommented for low precision modes, commented for high
precision modes
```

```
#for (i=1;i<=numFreq;i+=3) {
#  for (j=1;j<=numAtoms;j++) {
#     getline < "tempmodes"
#     mode[i,j,1]=$3
#     mode[i,j,2]=$4
#     mode[i,j,3]=$5
#     mode[i+1,j,1]=$6
#     mode[i+1,j,2]=$7
#     mode[i+1,j,3]=$8
#     mode[i+2,j,1]=$9
#     mode[i+2,j,2]=$10
#     mode[i+2,j,3]=$11
#     }
#  }
for (i=1;i<=numFreq;i++) {
#  print mode[i,1,1],mode[i,1,2],mode[i,1,3]
   }

#convert freqs to units used in spreedsheat, pick a random number,
#and decide vibrational quantum state and energy
srand()
# want to read from temp811, starting at a random place
tester=rand()*1000
for (i=1;i<=tester;i++) {
   getline < "temp811"
   }
for (i=1;i<=numFreq;i++) {
   getline < "temp811"
   randArr[i]=$1
   getline < "temp811"
   randArrB[i]=$1
   getline < "temp811"
   randArrC[i]=$1
}
# for a QM distribution for a harmonic oscillator in its ground state, we want to generate
a set of random numbers
#between -2 and 2 weighted such that numbers toward the center are properly more
common
i=1
while (i<=numFreq) {
   getline < "temp811"
   tempNum=2*($1-.5)
   prob=exp(-(tempNum^2))
   getline < "temp811"
```

```
  if ($1<prob) {
    randArrD[i]=tempNum
    i++
    }
  }

for (i=1;i<=numFreq;i++) {
  zpeJ[i]=0.5*h*c*freq[i]
  zpeK[i]=zpeJ[i]*avNum*0.239/1000
#program so that if the temp is too low, it just acts like 0 K
  if (temp<10) {
    vibN[i]=0
    }
  if (temp>=10) {
    zpeRat[i]=exp((-2*zpeK[i])/(0.001987*temp))
#if classical, treat as modes spaced by 10 wavenumbers
    if (classical==1) {
      Espace=0.5*h*c*10*avNum*0.239/1000
      zpeRat[i]=exp((-2*Espace)/(0.001987*temp))
      }
    Q[i]=1/(1-zpeRat[i])
    newRand=randArr[i]
#    print newRand
    vibN[i]=0
    tester=1/Q[i]
#    2008 updated line below to get up to 300 excitations of low modes
    for (j=1;j<=(300*zpeRat[i]+2);j++) {
      if (newRand>tester) vibN[i]++
      tester=tester+((zpeRat[i]^j)/Q[i])
      }
    }
  }

# figure out mode energies and maximum classical shift and then
# actual shift
for (i=1;i<=numFreq;i++) {
  modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i]+1)
  if (classical==1) modeEn[i]=(0.5*h*c*10*1E18)*(2*vibN[i])
# no 1/2 hv for imaginary frequencies
# treating modes with frequencies <10 as translations, ignoring their zero point energies
  if (freq[i]<10) modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i])
  maxShift[i]=(2*modeEn[i]/frc[i])^0.5
  if (initialDis==2) shift[i]=maxShift[i]*randArrD[i]
  if (initialDis==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
```

```
  if (initialDis==0) shift[i]=0
# no displacements along imaginary frequencies and very low ones - it is better to treat
these
# as translations - employing a shift can give you initial weird geometries
  if (freq[i]<10) shift[i]=0
  if (numimag==1) shift[1]=0
  if (numimag==2) shift[2]=0
  }
for (i=1;i<=numFreq;i++) {
#   print zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i]
  }

# multiply each of the modes by its shift and add them up
for (i=1;i<=numFreq;i++) {
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      shiftMode[i,j,k]=mode[i,j,k]*shift[i]
      geoArr[j,k]=geoArr[j,k]+shiftMode[i,j,k]
      }
    }
  }

#output the new geometry.
for (j=1;j<=numAtoms;j++) {
  print atSym[j],geoArr[j,1],geoArr[j,2],geoArr[j,3],atWeight[j]
  }

#now start toward velocities
for (i=1;i<=numFreq;i++) {
  kinEn[i]=100000*(modeEn[i]-0.5*frc[i]*shift[i]^2)
  vel[i]=(2*kinEn[i]/(redMass[i]/avNum))^0.5
#it is tricky here to set the velocities for modes along reaction coordinate
#I think I would like to have them all going the same direction, but setting
#the right direction is difficult.  I guess the thing to do is pick one direction
#and go with it, and if there is a problem the program will have to be changed here.
#use searchdir in progdyn.conf to change directions
#fixed this with numimag to allow for ground state dynamics and systems with two
imaginary frequencies
#when two, only the lowest one is sent in the searchdir direction, other is sent in random
direction
  if (numimag>1) numimag=1
  if (i>numimag) {
    if (randArrB[i]<0.5) vel[i]=-vel[i]
    }
```

```
  if (i==numimag) {
    if (searchdir=="negative") vel[i]=-vel[i]
    }
#   print vel[i]
  }

# multiply each of the modes by its velocity and add them up
for (i=1;i<=numFreq;i++) {
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      velMode[i,j,k]=mode[i,j,k]*vel[i]*timeStep
      velArr[j,k]=velArr[j,k]+velMode[i,j,k]
      }
    }
  }

#output the velocities.  The markers let a later program grab these velocities.
for (j=1;j<=numAtoms;j++) {
  print velArr[j,1],velArr[j,2],velArr[j,3]
  }

#anything else I add to the file is not going to be read but will be useful
#for error checking
for (i=1;i<=numFreq;i++) {
  if (initialDis<1.5) print randArr[i],vibN[i],vel[i]
  if (initialDis==2) print randArr[i],randArrD[i],vibN[i],vel[i]
  }
print "temp ",temp
print "initialDis",initialDis
print "timeStep",timeStep
print "numimag",numimag

}
```

3. Program prog1stpoint

```
BEGIN {
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point
unaffected by box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation
# this program creates the first input file for g03
# the title should be changed as appropriate
# the isomer number comes from a file isomernumber
```

```
#initialization
atomnumber=0

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag==1) print "***************** starting prog1stpoint *****************" >>
"diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

getline < "isomernumber"
isomernum = $1
```

```
print "%nproc=" processors
print "%mem=" memory
print "%chk=" checkpoint
print "#p " method " force scf=(tight,nosym) "
#print "IOp(3/76=0572004280)" #for mPW1K in g03
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
print ""
# make the title four words exactly, leaving out spaces if necessary
print title1,title2,title3,title4
print "runpoint 1"
print "runisomer ", isomernum
print ""
print charge,multiplicity
}

(/C / || /H / || /O / || /N / || /B / || /F / || /Cl / || /Al /) {
  atomnumber++
  printf("%s %.7f %.7f %.7f",$1,$2,$3,$4)
  if (atomnumber>highlevel) printf(" %s","M")
  print ""
  }

END {
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
print ""
}
```

4. Program prog2ndpoint

```
BEGIN {
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point
unaffected by box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 9, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation
```

```
# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag==1) print "***************** starting prog2ndpoint ****************" >>
"diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

# TO DO : move timestep to progdyn.conf
i=1;j=1;k=1
timestep=1E-15
avNum=6.02E23

#get the isomer number from file
```

```
getline < "isomernumber"
isomernum = $1

print "%nproc=" processors
print "%mem=" memory
print "%chk=" checkpoint
print "#p " method " force scf=(tight,nosym) "
#print "IOp(3/76=0572004280)" #for mPW1K in g03
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes
faster, sometimes not
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
print ""
# make the title four words exactly, leaving out spaces if necessary
print title1,title2,title3,title4
print "runpoint 2"
print "runisomer ", isomernum
print ""
print charge,multiplicity

# ok, now we have to figure the second point.  this should be
# x(t) = x + v*t + 1/2*F*t^2/m
# so we need to set up arrays for position, velocity, and force
getline < "geoPlusVel"
numAtoms=$1
# first the geometry
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  weight[i]=$5
  atSym[i]=$1
  for (j=1;j<=3;j++) {
    geoArr[i,j]=$(1+j)
    }
  }
#now we go ahead and add the velocities
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  for (j=1;j<=3;j++) {
    arr[i,j]=$j+geoArr[i,j]
    }
#   print arr[i,1],arr[i,2],arr[i,3]
  }
# first end the BEGIN
```

```
}
# now we go ahead and translate the forces and add them
(/         1    / || /         5    / || /         6    / || /         7    / || /         8    / || /         9    / || /
13    / || /         17    /) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j)
  }
#   print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]
}

END {
# turn the forces into motion
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {

forceArr[i,j]=0.5*1E10*forceArr[i,j]*627.509*(4184/(0.5292*avNum))*1E10*(timestep
^2)/(weight[i]/(avNum*1000))
     arr[i,j]=arr[i,j]+forceArr[i,j]
# if atoms are fixed, replace calcd new position by original position
     if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4))
arr[i,j]=geoArr[i,j]
     }
#   print forceArr[i,1],forceArr[i,2],forceArr[i,3]
  printf("%s %.7f %.7f %.7f",atSym[i],arr[i,1],arr[i,2],arr[i,3])
  if (i>highlevel) printf(" %s","M")
  print ""
  }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
print ""
}
```

5. Program progdynb

```
BEGIN { #this is the main routine for generating new .com files by the Verlet
algorithym
```

```
# May 2008 added option to put out velocities in vellist - make diag=2
# version Feb 2008 incorporates methodfile, boxon and boxsize
# version Jan 2008 incorporates fixed atoms, oniom, and velocity damping
# version August 2007 incorporates keepevery to decrease size of dyn file
# version Sept 11, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation

OFS="     ";i=1;j=1;k=1
# TO DO - move timestep to progdyn.conf
timestep=1E-15
avNum=6.02E23
#allow for damping from file named damping, but limit its range
damping=1
getline < "damping"
if (($1>0.05) && ($1<2.1)) damping=$1

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="keepevery") keepevery=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="boxon") boxon=$2
  if ($1=="boxsize") boxsize=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
```

```
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag==1) print "***************** starting progdynb *****************" >>
"diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

# get number of atoms and weights from geoPlusVel
getline < "geoPlusVel"
numAtoms=$1
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  weight[i]=$5
  atSym[i]=$1
  }

for (at=1;at<=numAtoms;at++) {
  getline < "old"
  oldarr[at,1]=$4
  oldarr[at,2]=$5
  oldarr[at,3]=$6
  }

for (at=1;at<=numAtoms;at++) {
  getline < "older"
  olderarr[at,1]=$4
  olderarr[at,2]=$5
  olderarr[at,3]=$6
  }

# record atom velocities for IVR analysis.  This is actually the velocity in the previous
run, which is the easiest to calculate.
getline < "isomernumber"
isomernum = $1
getline < "runpointnumber"
runpointnum = $1
if (diag==2) print "runpoint ",runpointnum-1,"runisomer ",isomernum >> "vellist"
for (at=1;at<=numAtoms;at++) {
```

```
  atomVel=((oldarr[at,1]-olderarr[at,1])^2 + (oldarr[at,2]-olderarr[at,2])^2
+(oldarr[at,3]-olderarr[at,3])^2)^.5
if (diag==2) print atomVel >> "vellist"
  }
}

#must adjust next line for weird atoms
(/         1    / || /         5    / || /         6    / || /         7    / || /         8    / || /         9    / || /
13    / || /        17    /) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j)
  }
#  print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]
}

END {
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {

forceArr[i,j]=1E10*forceArr[i,j]*627.509*(4184/(0.5292*avNum))*1E10*(timestep^2)/
(weight[i]/(avNum*1000))
    arr[i,j]=arr[i,j]+forceArr[i,j]
    }
  }
if ((runpointnum % keepevery)==0) system("cat g03.log >> dyn")
print "%nproc=" processors
print "%mem=" memory
print "%chk=" checkpoint
print "# " method " force scf=(maxcycle=200) "
#print "IOp(3/76=0572004280)" #for mPW1K in g03
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes
faster, sometimes not
print "pop=none "
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
#print "pop=none IOP(2/9=10,6/12=2)" #old IOPs for g98
print ""
print  title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ",isomernum
print ""
print charge,multiplicity
```

```
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {
    newarr[i,j]=oldarr[i,j]+damping*(oldarr[i,j]-olderarr[i,j])+forceArr[i,j]
    if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4))
newarr[i,j]=oldarr[i,j]
#turn around atoms outside the box
    if (boxon==1) {
      if (newarr[i,j]>boxsize) {
        if (oldarr[i,j]>olderarr[i,j]) newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-
oldarr[i,j])+forceArr[i,j]
        }
        if (newarr[i,j]<-1*boxsize) {
        if (oldarr[i,j]<olderarr[i,j]) newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-
oldarr[i,j])+forceArr[i,j]
        }
      }
    }
  printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3])
  if (i>highlevel) printf(" %s","M")
  print ""
  }
  print ""
  if (length(meth5)>2) print meth5
  if (length(meth6)>2) print meth6
  if (methodfilelines>=1) {
    for (i=1;i<=methodfilelines;i++) {
      getline < "methodfile"
      print $0
      }
    }
  print ""
}
```

6. Program randgen

```
# c program
# this can be replaced by a more reliable random number
# generator when available on a system
#include <stdio.h>
#include <stdlib.h>

int a,b,c;
double d;
```

```
int product(int x, int y);

int main(void)
{
  int count=1;
  srand48(time (0));
  while (count<=10000)
  {
    d = drand48();
    printf ("%.20f\n", d);
    count++;
  }
  return 0;
}
```

7. Program proganal

```
# pronounced pro-ganal
# this program requires serious rewriting for each new molecule
# or for reordered atoms, in order to pull out distances of interest
# revised from file used late 2005 and early 2006, getting dyns into separate files
# and adding extra functions
BEGIN {
getline < "isomernumber"
isomer=$1
}

/ BH3 Propene/ {
  printf("%s %s %s %s %s %s   ",$1,$2,$3,$4,$6,$8)
  runpoint=$6
  }
/   1  C    0.000000/,/     6  H    0.000000/ {
  if ($1==4) {
    C2B=$4
    C3B=$5
    }
  if ($1==10) {
    C2H10=$4
    C3H10=$5
    }
  if ($1==11) {
    C2H11=$4
    C3H11=$5
    }
```

```
  if ($1==12) {
    C2H12=$4
    C3H12=$5
    }
  }
END {
    printf("%s %.4f %s %.4f %s %.4f %s %.4f %s %.4f %s %.4f %s %.4f %s %.4f
","C2B",C2B,"C3B",C3B,"C2H10",C2H10,"C3H10",C3H10,"C2H11",C2H11,"C3H11"
,C3H11,"C2H12",C2H12,"C3H12",C3H12)
    if (runpoint>5000) {
      print "Too many points.  XXXX"
      movedyn(isomer)
      }
    if ((C2B<1.6) && (C3H10<1.1)) {
      print "Markovnikov with H10 XXXX"
      movedyn(isomer)
      }
    if ((C2B<1.6) && (C3H11<1.1)) {
      print "Markovnikov with H11 XXXX"
      movedyn(isomer)
      }
    if ((C2B<1.6) && (C3H12<1.1)) {
      print "Markovnikov with H12 XXXX"
      movedyn(isomer)
      }
    if ((C3B<1.6) && (C2H10<1.1)) {
      print "antiMarkovnikov with H10 XXXX"
      movedyn(isomer)
      }
    if ((C3B<1.6) && (C2H11<1.1)) {
      print "antiMarkovnikov with H11 XXXX"
      movedyn(isomer)
      }
    if ((C3B<1.6) && (C2H12<1.1)) {
      print "antiMarkovnikov with H12 XXXX"
      movedyn(isomer)
      }
    if ((C3B>9.0) && (C2B>9.0)) {
      print "bounced away to SM fast XXXX"
      movedyn(isomer)
      }
    if ((C3B>8.0) && (C2B>8.0) && (runpoint>200)) {
      print "bounced away to SM slow XXXX"
      movedyn(isomer)
```

```
      }
  system("date")
  }

function movedyn(isomer) {
  if (isomer==1) system("mv dyn dyn1")
  if (isomer==2) system("mv dyn dyn2")
  if (isomer==3) system("mv dyn dyn3")
  if (isomer==4) system("mv dyn dyn4")
  if (isomer==5) system("mv dyn dyn5")
  if (isomer==6) system("mv dyn dyn6")
  if (isomer==7) system("mv dyn dyn7")
  if (isomer==8) system("mv dyn dyn8")
  if (isomer==9) system("mv dyn dyn9")
  if (isomer==10) system("mv dyn dyn10")
  if (isomer==11) system("mv dyn dyn11")
  if (isomer==12) system("mv dyn dyn12")
  if (isomer==13) system("mv dyn dyn13")
  if (isomer==14) system("mv dyn dyn14")
  if (isomer==15) system("mv dyn dyn15")
  if (isomer==16) system("mv dyn dyn16")
  if (isomer==17) system("mv dyn dyn17")
  if (isomer==18) system("mv dyn dyn18")
  if (isomer==19) system("mv dyn dyn19")
  if (isomer==20) system("mv dyn dyn20")
  if (isomer==21) system("mv dyn dyn21")
  if (isomer==22) system("mv dyn dyn22")
  if (isomer==23) system("mv dyn dyn23")
  if (isomer==24) system("mv dyn dyn24")
  if (isomer==25) system("mv dyn dyn25")
  if (isomer==26) system("mv dyn dyn26")
  if (isomer==27) system("mv dyn dyn27")
  if (isomer==28) system("mv dyn dyn28")
  if (isomer==29) system("mv dyn dyn29")
  if (isomer==30) system("mv dyn dyn30")
}

function killdyn(isomer) {
  system("rm -f dyn")
}
```

8. progdyn.conf

```
#conf file for dynamics.  This is read by awk programs prog1stpoint, prog2ndpoint, and progdynb.
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.  You can add to these comments but
#don't use keywords as the first word on a line.  Don't delete lines - the program
#has no built in default values if they aren't here.
#values here are read repeatedly and can be changed in the middle of runs
method ONIOM(B3LYP/6-31G*:AM1)
method2 restricted #The options here are restricted, unrestricted, and read.
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things faster, sometimes not.
charge 0
multiplicity 1
memory 200000000
checkpoint dyn17.chk #uses one checkpoint file repeatedly
processors 1
diagnostics 0 # 1 prints out extra stuff to a file "diagnostics"
title BH3propene18THF classical VTSequil 298nodis # the title must be exactly four words
initialdis 0
timestep 1E-15
scaling 1.0
temperature 298.15
#add extra lines to .com files to implement things like the iop for mPW1k
#Leave the second word blank if you are not going to use them. otherwise any word you put in will end up in the com file
#only a single term with no spaces can be added, one per method line
#method3 IOp(3/76=0572004280)
#add the line below with big structures to get it to put out the distance matrix and the input orientation
method3 iop(2/9=2002)
method4
#method5 and method6 are placed at the end of the file instead of in the keyword section
method5
method6
#for more complicated ends of .com files, it will be necessary to put the ends in a file
#methodfile 6
#searchdir says what direction to follow the mode associated with the imaginary frequency.
#put as values the words "negative" or "positive"
searchdir negative
```

```
#for quassiclassical dynamics, the default, use 0.  for classical dynamics, use 1 below
classical 1
#line below gives number of negative frequencies - if 0, treats as ground state and
direction of all modes is random
#if 1, negative freq will go direction of searchdir
#if 2, only lowest freq will go direction of searchdir and other imag mode will go in
random direction
numimag 0
# the line below tells progdynb how often to write g03.log to file dyn, after the first two
points.  Use 1 for most dynamics
# until excessive, but use a higher integer if doing long term classical dynamics.
keepevery 10
# for ONIOM jobs, the following line states the number of highlevel atoms, which must
come before the medium level atoms
# make this number 999 if not ONIOM
highlevel 13
#use fixedatom1, fixedatom2, fixedatom3, fixedatom4 to fix atoms in space.
#note that fixing one atom serves no useful purpose and messes things up, while
#fixing two atoms fixes one distance, and
#fixing three has the effect of fixing three distances, not just two
#in current form fixed atoms only are meant to work with no displacements, that is,
initialdis=0
fixedatom1 3
fixedatom2 10
#fixedatom3 14
#dynamics with solvent molecules tends to blast molecules away.  Because of this,
#it would be good to have a pressure and periodic boundary conditions, etc, but until
#I learn how to do this, I can just restrict the molecules to a box
#atoms outside this box get bounced.  Set box size so as to fit the entire initial molecule
but not have too much extra room
#the box does not affect anything until progdynb
boxon 1
boxsize 7.5
#to be implemented:
rotation 0 #use 1 to turn on rotational modes
#since displacements run into a problem with easy rotation modes such as a methyl
group,
#it would be easy to turn off displacements for particular modes.  Sometimes this would
be
#the right thing to do but it would be awkward to explain it in a paper.
numberlimitedmodes 0
limitedmodes 3 5
```

#updated Aug 9, 2007 to include the possibility of classical dynamics by the keyword classical
#updated Jan 2008 to include fixed atoms, ONIOM jobs, keepevery, and box size
#update Feb 2008 to include methodfile parameter

VITA

Yatsandra Oyola

Mailing address:
PO Box 2474
Bayamon, PR 00960

Phone: 979-224-6054 (cell)
E-mail: yoyola@mail.chem.tamu.edu
yal_oyola@hotmail.com

EDUCATION

Ph.D., Chemistry
Department of Chemistry, **Texas A&M University, College Station, Texas**
December 2010

B.S., Chemistry, *Magna Cum Laude*
Department of Chemistry, **Unversity of Puerto Rico, San Juan, Puerto Rico**
June 2004

RESEARCH EXPERIENCE

2006-2010 **Department of Chemistry, Texas A&M University**, College Station, TX
Advisor: Prof. Daniel Singleton; *Graduate Research Assistant*
- Determination of dynamic effects in hydroboration reactions.

2004-2006 **Department of Chemistry, Texas A&M University**, College Station, TX
Advisor: Prof. Daniel Romo; *Graduate Research Assistant*
- Utilization of β-lactone chemistry for the synthesis of fatty acid synthase (FAS) inhibitors.
- Synthesis of activity-based proteomic probes: Identification of tetrahydrolipstatin derivatives as antagonist of FAS.

June - August 2004 **Bristol-Myers Squibb Company**, Barceloneta, Puerto Rico
Chemical Development Area, Laboratory for Process Development.
- Summer Associate – Analysis and validation of experimental procedures

June – August 2003 **Pfizer Global Research and Development**, Groton Connecticut,
Research and Development Department.
- Summer Associate – Scope and reactivity of unusual products from the Fisher-Indole reaction

2001-2004 **Department of Chemistry, University of Puerto Rico,** San Juan**,** PR
Advisor: John A. Soderquist; *Undergraduate Research Assistant*.
- Suzuki-Miyaura cross-coupling reactions via hydroboration of